SUPPORTING INFORMATION

Synthesis of α-CF_3-proline derivatives by means of a formal (3+2)-cyclisation between trifluoropyruvate imines and Michael acceptors

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1. General Information:

1.1. General Methods

^{1}H- and ^{13}C-NMR spectra were recorded on a Bruker Avance III 300 MHz spectrometer with a broad band observe probe and a sample changer for 16 samples, on a Bruaker Avance DRX 500 MHz spectrometer, and on a Bruker Avance III 700 MHz spectrometer with an Ascend magnet and TCI cryoprobe, which are both property to the Austro-Czech NMR-Research Center "RERI-uasb". All NMR spectra were referenced on the solvent peak. High resolution mass spectra were obtained using an Agilent 6520 Q-TOF mass spectrometer with an ESI source and an Agilent G1607A coaxial sprayer or a Thermo Fisher Scientific LTQ Orbitrap XL with an Ion Max API Source. Analyses were made in the positive ionization mode if not otherwise stated. Purine (exact mass for $[M+H]^+$ = 121.050873) and 1,2,3,4,5,6-hexakis(2,2,3,3-tetrafluoropropoxy)-1,3,5,2,4,6-triaza-triphosphinane (exact mass for $[M+H]^+$ = 922.009798) were used for internal mass calibration.

Preparative column chromatography was carried out using Davisil LC 60A 70-200 MICRON silica gel. TLC probes were detected at 254 nm or stained with with an appropriate staining solution (compare section 3.1.3).

HPLC was performed using a Dionex Summit HPLC system with a Chiralcel YMC-SB (250 x 4.6 mm, 5 µm) chiral stationary phase.

All chemicals were purchased from commercial suppliers and used without further purification unless otherwise stated. All reactions were carried out under Argon.

The acceptors **6a-k** and **7** are literature known and were synthesized as described previously.[1,2]

[1] C.J. Lee, C.N. Sheu, C.C. Tsai, Z.Z. Wu, W. Lin, *Chem. Commun.* **2014**, 50, 5304-5306.
[2] P. Bobal, J. Bobalova, *Molecules* **2013**, *18*, 2212-2221.

1.2. X-Ray Analysis

X-ray quality crystals were selected in Fomblin® Y H-VAC 140/13 perfluoropolyether at ambient temperature. The data was collected at 296(2) K on a *Bruker* ***D8 Quest Eco*** diffractometer using graphite monochromated Mo K_α radiation (λ = 0.71073 Å). The data was processed using APEX3,[3] the structures were solved by intrinsic phasing (XT, Version 2014/5),[4] and refined by full matrix least squares procedures on F^2 (SHELXL, Version 2014/7)[5] using the graphical interface Shelxle[6] within the SHELXTL suite of programs by Bruker. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were calculated geometrically, and a riding model was applied in the refinement process.

CCDC 1911986 contains the supplementary crystallographic data for compound **5b**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre at www.ccdc.cam.ac.uk.

[3] Bruker (2016), *APEX3 v2016.9-0*, *SAINT V8.37A*, *SHELXTL-2014*, Bruker AXS Inc.: Madison (WI), USA, **2016**.

[4] a) G. M. Sheldrick, *SHELXT-2014: Program for the Solution of Crystal Structures*, University of Göttingen, Germany, **2014**. b) G. M Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.* **2008**, *64*, 112−122. c) G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Adv.* **2015**, *71*, 3−8.

[5] a) G. M. Sheldrick, *SHELXL-2014: Program for the Refinement of Crystal Structures*, University of Göttingen, Germany, **2014**. b) G. M. Sheldrick, *Acta Crystallogr., Sect. C: Struct. Chem.* **2015**, *71*, 3−8.

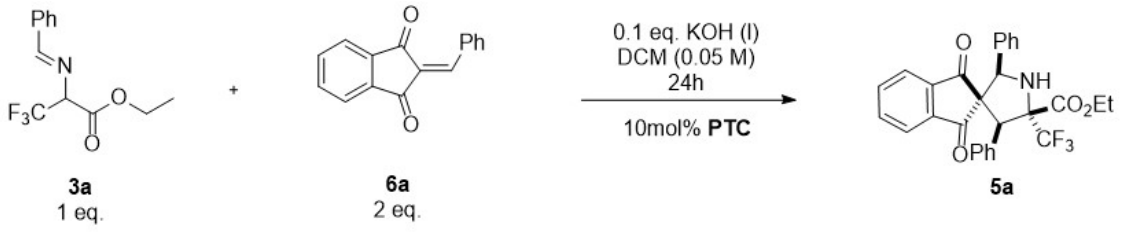
[6] C. B. Hübschle, G. M. Sheldrick, B. Dittrich, *Shelxle: a Qt graphical user interface for SHELXL*, *J. Appl. Crystallogr.* **2011**, *44*, 1281−1284.

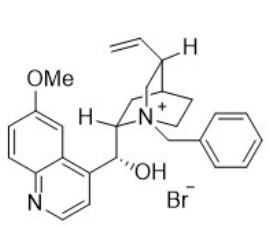
Table 1. Crystal data, data collection and structure refinement details for compound **5b**.

Compound	**5b**
Empirical formula	$C_{28}H_{21}BrF_3NO_4$
Formula weight [g/mol]	572.37
Color	colorless
Crystal size [mm]	0.44 × 0.37 × 0.27
Crystal system	triclinic
Space group	*P−1*
a [Å]	10.1546(3)
b [Å]	10.8743(4)
c [Å]	13.3084(5)
α [°]	85.375(2)
β [°]	77.474(1)
γ [°]	63.999(1)
V [Å^3]	1289.22(8)
Z	2
D_{calc} [g/cm^3]	1.474
μ [mm^{-1}]	1.65
T [K]	296
θ range [°]	2.6-23.9
No. of reflections measured	110108
No. of independent reflections	4719
Obs. Reflections with $I > 2\sigma(I)$	3229
No. of Parameters refined/restraints	339/1
Absorption correction	multi-scan
T_{min}, T_{max}	0.58, 0.66
$\Delta\rho_{min}/\Delta\rho_{max}$ [e Å^{-3}]	−0.35/0.38
F(000)	580
R_{int}	0.125
R_1 ($R[F^2 \geq 2\sigma(F^2)]$)	0.047
wR_2 ($wR(F^2)$)	0.106
GooF	1.13
CCDC no.	1911986

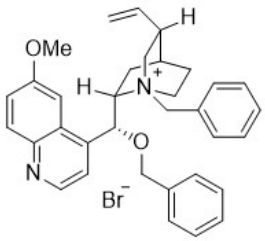
2. Asymmetric Phase-Transfer Catalysts

2.1 Screening of Different Phase-Transfer Catalysts [7,8,9]

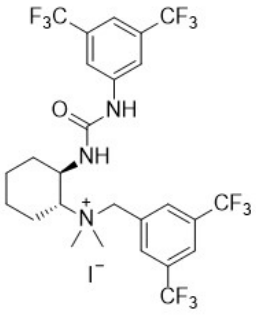




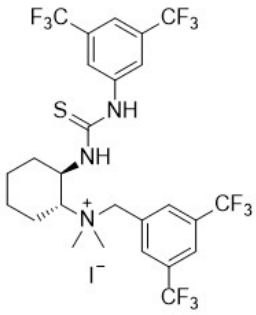
PTC 1
conv: >99%; yield: 65%
dr 65:27:7:1; ee 24%



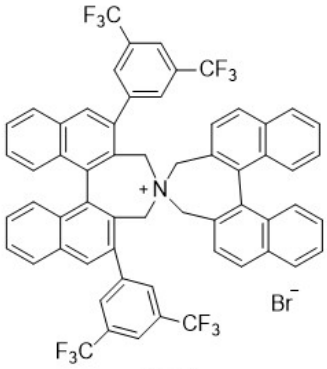
PTC 2
conv: 79%; yield: 31%
dr 79:15:5:1; ee 2%



PTC 3
conv: 73%; yield: 46%
dr 70:13:15:2; ee 14%



PTC 4
conv: 77%; yield: 48%
dr 85:3:10:2; ee 6%



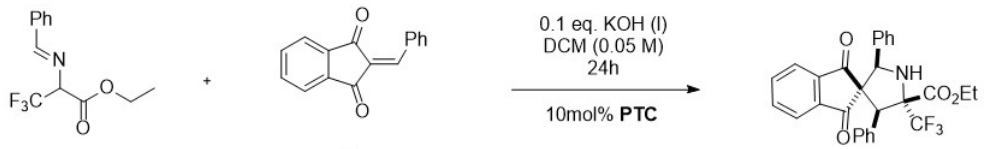
PTC 5
conv: 77%; yield: 48%
dr 85:3:10:2; ee 6%

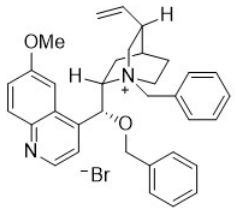
[7] For early reports on Cinchona-based PTCs: (a) R. Helder, J. C. Hummelen, R. W. P. M. Laane, J. S. Wiering and H. Wynberg, *Tetrahedron Lett.*, **1976**, 17, 1831. (b) U. H. Dolling, P. Davis and E. J. J. Grabowski, *J. Am. Chem. Soc.* **1984**, 106, 446.

[8] For the seminal report on Maruoka-type catalysts: T. Ooi, M. Kameda and K. Maruoka*, J. Am. Chem. Soc.* 1999, **121**, 6519.

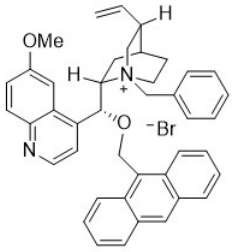
[9] For cyclohexane diamine-based bifunctional ammonium salts: (a) J. Novacek and M. Waser, Eur. J. Org. Chem. **2014**, 802. (b) M. Tiffner, J. Novacek, A. Busillo, K. Gratzer, A. Massa, and M. Waser *RSC Adv.*, **2015**, *5*, 78941.

2.2 Further Cinchona Alkaloid Catalyst Screening

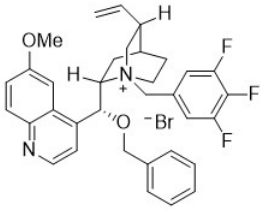




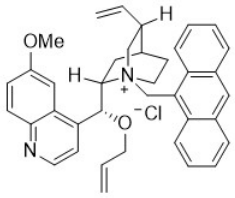
PTC 2
conv: 79%; yield: 31%
dr 79:15:5:1; ee 2%



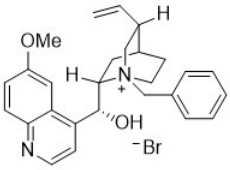
PTC 6
conv: 65%; yield: 52%
dr 81:12:6:1; ee 2%



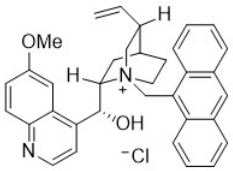
PTC 7
conv: 56%; yield: 35%
dr 86:7:6:1; ee 2%



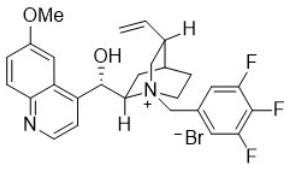
PTC 8
conv: 74%; yield: 47%
dr 76:18:5:1; ee 2%



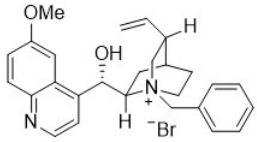
PTC 1
conv: >99%; yield: 65%
dr 65:27:7:1; ee 24%



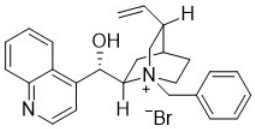
PTC 9
conv: >99%; yield: 62%
dr 59:34:6:1; ee 4%



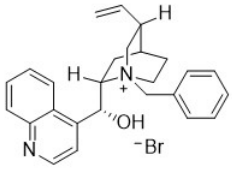
PTC 10
conv: >99; yield: 68%
dr 66:26:7:1; ee -10%



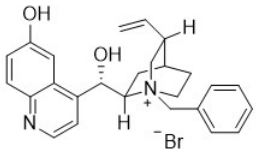
PTC 11
conv: >99; yield: 40%
dr 76:17:6:1; ee -16%



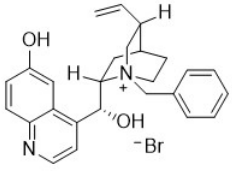
PTC 12
conv: >99; yield: 62%
dr 70:23:6:1; ee -4%



PTC 13
conv: >99; yield: 74%
dr 77:17:5:1; ee 14%



PTC 14
conv: 0%; yield: -
dr -; ee -



PTC 15
conv: >99; yield: 71%
dr 76:17:6:1; ee 4%

2.3 Reaction Condition Screening

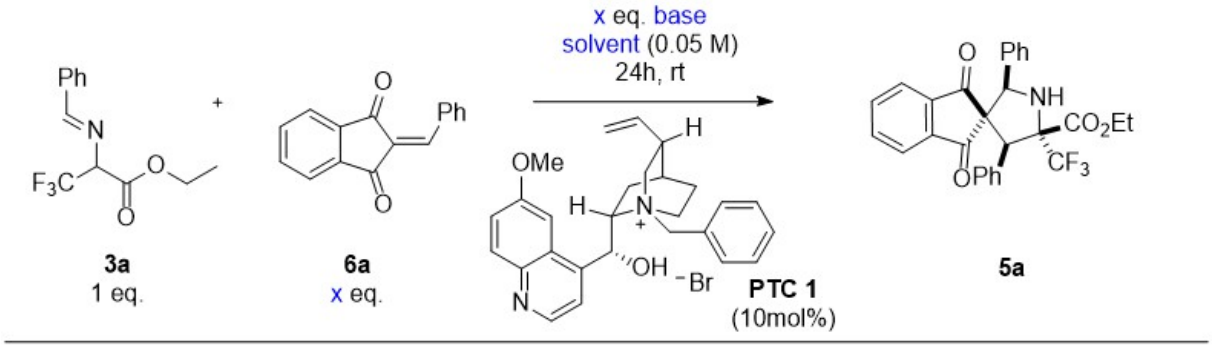
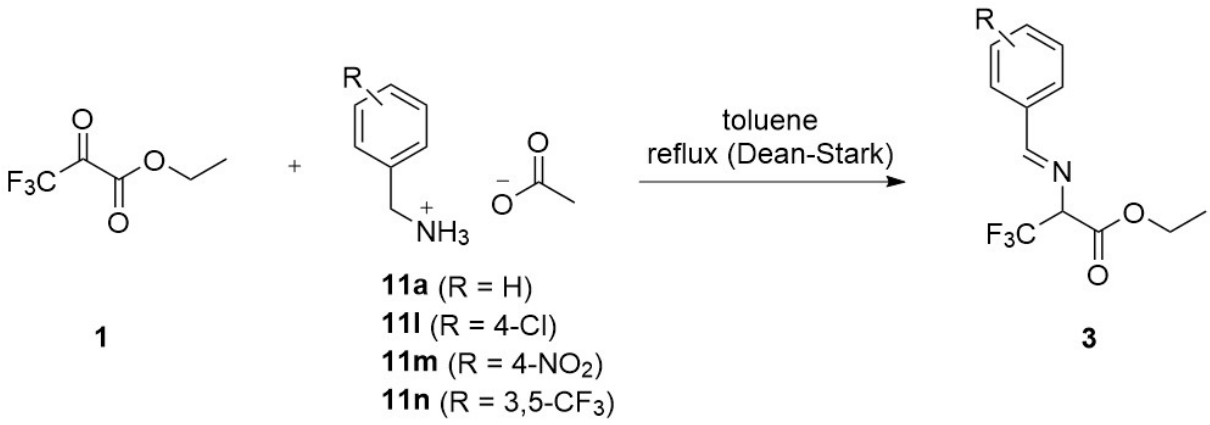


Table 2. Screening of the reaction conditions for the enantioselective (3+2)-cycloaddition of the azaallyl anion precursor **3a** and acceptor **6a**.

entry	eq. **6a**	solvent	base	base eq.	conv. [%]	yield [%]	d.r.	ee
1	1.2	**DCM**	aq. KOH (50%)	0.1	>99	69	58:34:7:1	16
3	1.2	**MeCN**	aq. KOH (50%)	0.1	>99	72	91:6:3:0	2
4	1.2	**THF**	aq. KOH (50%)	0.1	>99	78	68:23:8:1	10
5	1.2	**Et_2O**	aq. KOH (50%)	0.1	>99	65	86:10:3:1	10
6	1.2	**EtOAc**	aq. KOH (50%)	0.1	>99	70	77:17:6:0	16
7	1.2	**$CHCl_3$**	aq. KOH (50%)	0.1	53	22	79:11:9:1	16
8	1.2	**MTBE**	aq. KOH (50%)	0.1	>99	60	56:35:7:2	12
9	1.2	**dioxane**	aq. KOH (50%)	0.1	96	68	45:41:11:3	16
10	1.2	**1,2-DCE**	aq. KOH (50%)	0.1	>99	79	51:41:6:2	18
11	1.2	**cyclohexane**	aq. KOH (50%)	0.1	0	-	-	-
12	1.2	**toluene**	aq. KOH (50%)	0.1	20	16	65:20:13:2	-
13	2	DCM	aq. KOH (50%)	**1**	>99	52	91:6:3:0	14
14	2	DCM	aq. KOH (50%)	**10**	0	-	-	-
15	2	DCM	**aq. KOH (10%)**	0.1	59	25	74:18:7:1	8
16	2	DCM	**aq. KOH (25%)**	0.1	68	43	75:17:7:1	12
17	2	DCM	**aq. Cs_2CO_3 (50%)**	0.1	99	69	78:13:8:1	2
18	2	DCM	**DBU**	0.1	>99	71	92:2:5:1	4
19	2	DCM	**aq. K_2CO_3 (25%)**	0.1	98	65	86:6:8:0	6
20	2	DCM	**aq. K_3PO_4 (25%)**	0.1	93	78	83:8:8:1	8
21	2	DCM	**LiOH (s)**	1	>99	65	>99:0:0:0	6
22	2	DCM	**K_3PO_4 (s)**	0.1	99	80	75:17:7:1	6
23	2	DCM	**K_2CO_3 (s)**	0.1	>99	74	74:18:7:1	6
24	2	DCM	**Cs_2CO_3 (s)**	0.1	>99	70	63:30:6:1	12

3. Syntheses

3.1 Syntheses of Imines 3



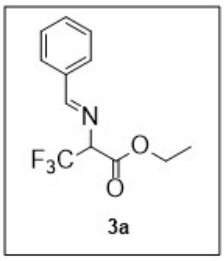
1

11a (R = H)
11l (R = 4-Cl)
11m (R = 4-NO_2)
11n (R = 3,5-CF_3)

3

General procedure 1: The synthesis was performed according to a modified literature procedure.[10] Acetic acid (10 mmol, 0.572 mL) was added to a stirred solution of benzylamine **11** (10 mmol) in 40 mL dry toluene at room temperature and the reaction mixture turned turbid/solid. Subsequently ethyl-3,3,3-trifluoropyruvate (**1**) (10 mmol, 1.33 mL) was added and the solution turned clear again. The reaction mixture was stirred at reflux under Dean-Stark conditions for 16 h. The crude product was purified by flash chromatography to yield the imines **3** in the reported yields.

3.1.1 Analytical Details of Imines 3



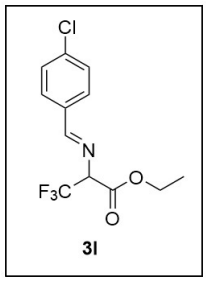
3a

3a: Compound was prepared according to the general procedure 1, starting from benzylamine **11a** (10 mmol, 1.10 mL) and give a yellow oil with an isolated yield of 55%.

HRMS (ESI): m/z calculated for $C_{12}H_{12}F_3NO_2$: 260.0898 $[M+H]^+$; found: 260.0896.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 8.40 (s, 1H), 7.86-7.82 (m, 2H), 7.51-7.41 (m, 3H), 4.52 (q, J = 7.3 Hz, 1H), 4.30 (q, J = 7.0 Hz, 2H), 1.32 (t, J = 7.5 Hz, 3H) ppm; ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -71.68 (d, J = 7.1 Hz, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 192.5, 169.0, 164.7, 134.9, 132.3, 129.9, 129.1, 128.9, 123.0 (q, J = 280.0 Hz), 73.5 (q, J = 29.5 Hz), 62.6, 14.1 ppm.

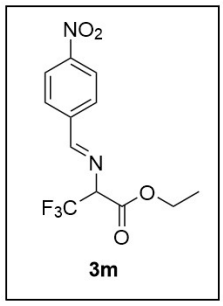
[10] H. Ohkura, D. O. Berbasov, V. A. Soloshonok, *Tetrahedron* **2003**, 59, 1647-1656.



3l: Compound was prepared according to the general procedure 1, starting from 4-chlorobenzylamine **11l** (10 mmol, 1.12 mL) and give a yellow oil with an isolated yield of 32%.

HRMS (ESI): *m/z* calculated for $C_{12}H_{11}ClF_3NO_2$: 294.0509 $[M+H]^+$; found: 294.0506.

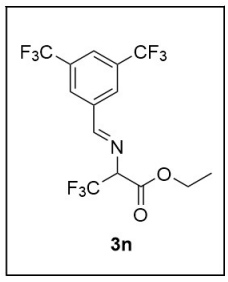
^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 8.35 (s, 1H), 7.81-7.69 (m, 2H), 7.47-7.31 (m, 2H), 4.53 (q, J = 7.0 Hz, 1H), 4.28 (q, J = 7.0 Hz, 2H), 1.29 (t, J = 7.5 Hz, 3H) ppm; ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -71.64 (d, J = 7.1 Hz, 3F) ppm.; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 190.9, 167.6, 164.5, 138.4, 130.9, 130.3, 129.5, 128.1, 122.7 (q, J = 281 Hz), 73.1 (q, J = 31 Hz), 62.6, 14.0 ppm.



3m: Compound was prepared according to the general procedure 1, starting from 4-nitrobenzylamine **11m** (10 mmol, 1.50 g) and give a yellow oil with an isolated yield of 35%. The commercial available 4-nitrobenzylamine hydrochloride was dissolved in 25% aq. ammonia solution and extracted three times with DCM. The organic phase was dried with Na_2SO_4, filtered and evaporated to dryness to get the 4-nitrobenzylamine.

HRMS (ESI): m/z calculated for $C_{12}H_{11}F_3N_2O_4$: 305.0749 $[M+H]^+$; found: 305.0747.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 8.50 (s, 1H), 8.32-8.29 (m, 2H), 8.04-8.01 (m, 2H), 4.61 (q, J = 7.0 Hz, 1H), 4.32 (q, J = 7.0 Hz, 2H), 1.33 (t, J = 7.5 Hz, 3H) ppm; ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -71.42 (d, J = 7.1 Hz, 3F) ppm.; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 190.2, 166.6, 164.0, 149.9, 139.9, 130.5, 129.8, 123.9, 122.3 (q, J = 281 Hz), 73.0 (q, J = 31 Hz), 62.8, 13.9 ppm.

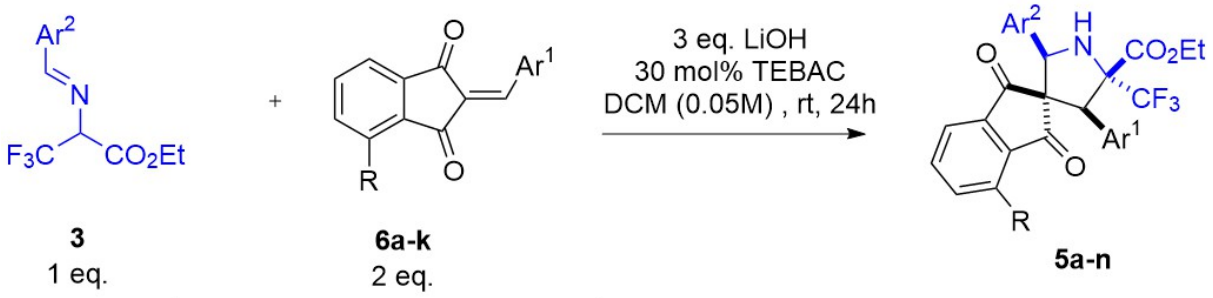


3n: Compound was prepared according to the general procedure 1, starting from 3,5-bis(trifluoromethyl)benzylamine **11n** (10 mmol, 1.78 mL) and give a yellow oil with an isolated yield of 33%.

HRMS (ESI): *m/z* calculated for $C_{14}H_{10}F_9NO_2$: 396.0646 $[M+H]^+$; found: 396.0640.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 8.51 (s, 1H), 8.28 (s, 2H), 7.99 (s, 1H), 4.61 (q, J = 7.3 Hz, 1H), 4.32 (dq, J_1 = 7.1 Hz, J_2 = 1.7 Hz, 2H), 1.33 (t, J = 7.5 Hz, 3H) ppm; ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -63.15 (s, 6H), -71.51 (d, J = 7.3 Hz, 3F) ppm.; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 165.9, 164.1, 136.7, 132.6 (q, J = 33.9 Hz), 129.0, 125.5, 123.3 (q, J = 270 Hz), 122.9 (q, J = 280 Hz), 72.9 (q, J = 29.6 Hz), 63.0, 14.0 ppm.

3.2 Formal (3+2)-Cycloaddition – Arylidene-Indandione



3
1 eq.

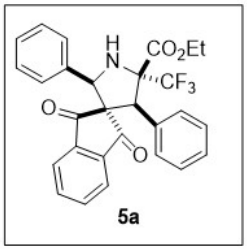
6a-k
2 eq.

5a-n

6a: Ar^1=C_6H_5, R=H
6b: Ar^1=4-Br-C_6H_4, R=H
6c: Ar^1=4-OMe-C_6H_4, R=H
6d: Ar^1=4-NO_2-C_6H_4, R=H
6e: Ar^1=4-Cl-C_6H_4, R=H
6f: Ar^1=4-C_6H_5-C_6H_4, R=H
6g: Ar^1=naphth-1-yl, R=H
6h: Ar^1=fur-2-yl, R=H
6i: Ar^1=thien-2-yl, R=H
6j: Ar^1=C_6H_5, R=F
6k: Ar^1=C_6H_5, R=NO_2

General procedure 2: To a stirred solution of the corresponding arylidene-indandione **6a-k** (0.2 mmol) in dry DCM (2 mL), LiOH (0.3 mmol, 7.2 mg), TEBAC (30 mol%, 0.03 mmol, 7.8 mg) and imine **3** (0.1 mmol) were added successively. The reaction mixture was stirred for 24 h at room temperature. The mixture was filtered over a pad of silica and washed with Et_2O. After evaporation of the solvent the product was purified by column chromatography with a gradient of heptanes and ethylacetate (20:1 – 10:1 – 5:1) to yield products **5a-n** with yields and diastereomeric ratios stated below.

3.2.1 Analytical Details of Proline Derivatives 5a-n



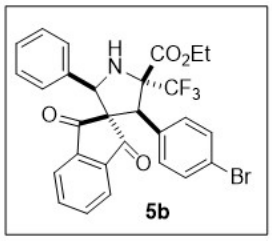
5a

5a: The reaction was performed according to the general procedure 2, with imine **3a** (1 mmol, 259.0 mg), arylidene-indandione **6a** (2 mmol, 468.0 mg), LiOH (3 mmol, 72.0 mg) and TEBAC (0.3 mmol, 78.1 mg). The product occurs as orange crystals with a melting range of 155.8-156.9 °C, an isolated yield of 98% and a dr of 100:0:0:0.

R_f: 0.82 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{28}H_{22}F_3NO_4$: 494.1574 $[M+H]^+$; found: 494.1580.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 7.76-7.73 (m, 1H), 7.60-7.52 (m, 3H), 7.15-7.06 (m, 10H), 4.93-4.83 (m, 2H), 4.65 (s, 1H), 4.31-4.20 (m, 1H), 3.96-3.86 (m, 1H), 0.94 (t, J = 7.1 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.22 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.4, 199.4, 166.7, 142.6, 142.1, 135.9, 135.6, 133.5, 133.5, 130.3, 128.4, 128.4, 128.2, 127.9, 126.7, 126.2 (q, J = 298 Hz), 124.1, 122.0, 122.9, 74.6 (q, J = 28 Hz), 72.1, 71.3, 63.0, 60.7, 14.2, 13.4 ppm.

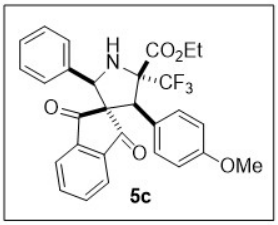


5b: The reaction was performed according to the general procedure 2, with imine **3a** (0.1 mmol, 25.9 mg) and arylidene-indandione **6b** (0.2 mmol, 62.6 mg). The product occurs as yellow crystals with a melting range or 119.2-123.1 °C, an isolated yield of 70% and a dr of 100:0:0:0.

R_f: 0.67 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{28}H_{21}BrF_3NO_4$: 572.0679 $[M+H]^+$; found: 572.0690.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 7.77-7.74 (m, 1H), 7.63-7.52 (m, 3H), 7.26-7.24 (m, 2H), 7.07-7.01 (m, 7H), 4.89-4.78 (m, 2H), 4.60 (s, 1H), 4.36-4.25 (m, 1H), 4.02-3.91 (m, 1H), 1.02 (t, J = 7.1 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.36 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.3, 199.0, 166.5, 142.4, 142.1, 142.1, 136.0, 135.8, 133.1, 132.6, 132.0, 131.5, 131.4, 128.4, 127.7, 126.5, 126.2 (q, J = 298 Hz), 123.0, 122.9, 122.5, 74.5 (q, J = 28 Hz), 72.1, 71.6, 63.2, 59.5, 13.5 ppm.

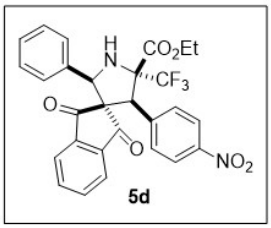


5c: The reaction was performed according to the general procedure 2, with imine **3a** (0.1 mmol, 25.9 mg) and arylidene-indandione **6c** (0.2 mmol, 52.8 mg). The product occurs as yellow oil with an isolated yield of 32% and a dr of 96:4:0:0.

R_f: 0.50 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{29}H_{23}F_3NO_5$: 524.1679 $[M+H]^+$; found: 524.1679.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 7.76-7.73 (m, 1H), 7.61-7.53 (m, 3H), 7.13-7.02 (m, 7H), 6.67-6.62 (m, 2H), 4.90-4.80 (m, 2H), 4.61 (s, 1H), 4.35-4.24 (m, 1H), 4.01-3.90 (m, 1H), 3.66 (s, 1H), 1.01 (t, J = 7.1 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.26 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.6, 166.8, 159.4, 142.7, 142.2, 135.9, 135.6, 133.7, 131.4, 128.5, 126.7, 126.4 (q, J = 298 Hz), 125.4, 123.0, 122.9, 113.7, 71.5 (q, J = 30 Hz), 63.0, 60.0, 55.2, 13.5 ppm.

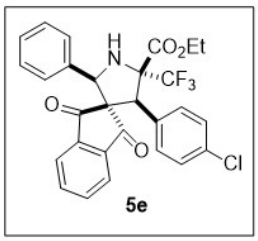


5d: The reaction was performed according to the general procedure 2, with imine **3a** (0.1 mmol, 25.9 mg) and arylidene-indandione **6d** (0.2 mmol, 55.8 mg). The product occurs as yellow crystals with a melting range of 100.8 -104.3°C, an isolated yield of 73% and a dr of 100:0:0:0.

R_f: 0.65 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{28}H_{20}F_3N_2O_6$: 539.1424 $[M+H]^+$; found: 539.1427.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 8.00-7.97 (m, 2H), 7.77-7.73 (m, 1H), 7.65-7.52 (m, 3H), 7.38-7.33 (m, 2H), 7.11-7.05 (m, 5H), 4.91-4.79 (m, 2H), 4.74 (s, 1H), 4.41-4.31 (m, 1H), 4.05-3.94 (m, 1H), 1.04 (t, J = 7.1 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.50 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.1, 198.4, 166.2, 147.8, 142.3, 141.9, 141.1, 136.3, 136.0, 132.8, 131.5, 128.8, 127.6, 125.8 (q, J = 284 Hz), 123.4, 123.1, 123.1, 74.3 (q, J = 34 Hz), 72.4, 72.1, 59.0, 13.6 ppm.

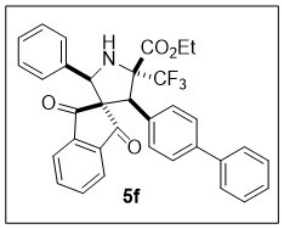


5e: The reaction was performed according to the general procedure 2, with imine **3a** (0.1 mmol, 25.9 mg) and arylidene-indandione **6e** (0.2 mmol, 53.6 mg). The product occurs as yellow oil with an isolated yield of 68% and a dr of 100:0:0:0.

R_f: 0.73 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{28}H_{20}ClF_3NO_4$: 528.1184 $[M+H]^+$; found: 528.1192.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 7.77-7.74 (m, 1H), 7.64-7.52 (m, 3H), 7.12-7.06 (m, 9H), 4.90-4.78 (m, 2H), 4.62 (s, 1H), 4.36-4.25 (m, 1H), 4.02-3.91 (m, 1H), 1.26 (t, J = 7.2 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.35 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.4, 199.1, 166.6, 142.5, 142.1, 142.1, 136.1, 135.8, 134.4, 133.2, 132.2, 131.8, 131.8, 128.6, 128.6, 128.5, 126.6, 126.2 (q, J = 298 Hz), 123.0, 123.0, 74.4 (q, J = 34 Hz), 72.2, 71.6, 63.2, 59.5, 13.5 ppm.

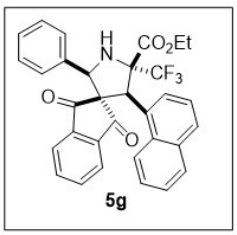


5f: The reaction was performed according to the general procedure 2, with imine **3a** (0.1 mmol, 25.9 mg) and arylidene-indandione **6f** (0.2 mmol, 62.0 mg). The product occurs as yellow oil with an isolated yield of 84% and a dr of 100:0:0:0.

R_f: 0.78 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{34}H_{26}F_3NO_4$: 570.1887 $[M+H]^+$; found: 570.1893.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 7.80-7.75 (m, 1H), 7.62-7.53 (m, 3H), 7.46-7.43 (m, 2H), 7.39-7.28 (m, 5H), 7.22-7.19 (m, 2H), 7.12-7.08 (m, 5H), 4.95-4.85 (m, 2H), 4.70 (s, 1H), 4.33-4.22 (m, 1H), 4.02-3.91 (m, 1H), 0.96 (t, J = 7.1 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.19 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.4, 199.3, 166.6, 142.5, 142.0, 140.8, 140.1, 135.8, 135.5, 133.3, 132.4, 130.6, 128.8, 128.3, 128.3, 127.5, 126.8, 126.8, 126.5, 125.7 (q, J = 285 Hz), 122.9, 122.8, 74.5 (q, J = 29 Hz), 72.1, 71.3, 63.0, 60.1, 13.3 ppm.

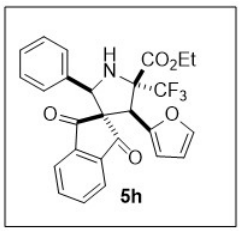


5g: The reaction was performed according to the general procedure 2, with imine **3a** (0.1 mmol, 25.9 mg) and arylidene-indandione **6g** (0.2 mmol, 56.8 mg). The product occurs as yellow crystals with a melting range of 160.4-162.3 °C, an isolated yield of 72% and a dr of 100:0:0:0.

R_f: 0.81 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{32}H_{24}F_3NO_4$: 544.1730 $[M+H]^+$; found: 544.1739.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 8.34 (d, 8.7 Hz, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.65-7.60 (m, 3H), 7.52-7.45 (m, 4H), 7.42-7.38 (m, 1H), 7.22-7.08 (m, 6H), 5.87 (s, 1H), 5.11-5.00 (m, 2H), 4.30-4.20 (m, 1H), 3.95-3.84 (m, 1H), 0.88 (t, J = 7.1 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -73.79 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.6, 199.5, 167.1, 142.8, 141.8, 135.8, 135.5, 134.1, 133.6, 132.3, 129.7, 128.9, 128.9, 128.4, 127.9, 127.2, 126.7, 126.1 (q, J = 284 Hz), 125.9, 124.3, 123.0,122.9, 122.8, 75.4 (q, J = 28 Hz), 72.6, 71.6, 63.1, 52.5, 13.4 ppm.

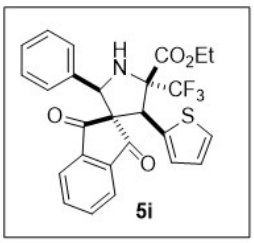


5h: The reaction was performed according to the general procedure 2, with imine **3a** (0.1 mmol, 25.9 mg) and arylidene-indandione **6h** (0.2 mmol, 44.8 mg). The product occurs as orange crystals with a melting range of 153.7-156.1 °C, an isolated yield of 61% and a dr of 100:0:0:0.

R_f: 0.67 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{26}H_{19}F_3NO_5$: 484.1366 $[M+H]^+$; found: 484.1371.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 7.80-7.78 (m, 1H), 7.66-7.56 (m, 3H), 7.11-7.07 (m, 6H), 6.14-6.11 (m, 2H), 4.87-4.74 (m, 3H), 4.33-4.23 (m, 1H), 4.11-4.00 (m, 1H), 1.10 (t, J= 7.3 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.98 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 198.9, 198.0, 166.1, 146.8, 142.6, 142.5, 141.9, 136.0, 135.5, 133.3, 128.5, 128.5, 126.7, 125.8 (q, J = 284 Hz), 123.0, 123.0, 110.7, 110.6, 73.2 (q, J = 33 Hz), 70.8, 69.3, 63.4, 52.5, 13.7 ppm.

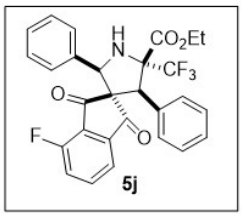


5i: The reaction was performed according to the general procedure 2, with imine **3a** (0.1 mmol, 25.9 mg) and arylidene-indandione **6i** (0.2 mmol, 48.0 mg). The product occurs as red crystals with a melting range of 147.1-150.2 °C, an isolated yield of 56% and a dr of 100:0:0:0.

R_f: 0.60 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{26}H_{20}F_3NO_4S$: 500.1138 $[M+H]^+$; found: 500.1143.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 7.79-7.76 (m, 1H), 7.65-7.55 (m, 3H), 7.11-7.05 (m, 5H), 7.04-7.02 (m, 1H), 6.89-6.88 (m, 1H), 6.80-6.77 (m, 1H), 5.00 (s, 1H), 4.88-4.79 (m, 2H), 4.31-4.20 (m, 1H), 4.03-3.92 (m, 1H), 1.02 (t, J= 7.2 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.20 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.4, 198.8, 166.2, 142.7, 142.3, 136.0, 135.6, 135.0, 133.2, 129.4, 128.6, 128.5, 126.8,, 126.6, 125.8, 125.4 (q, J = 284 Hz), 123.1, 123.0, 74.8 (q, J = 26 Hz), 71.8, 71.4, 63.3, 54.4, 13.5 ppm.

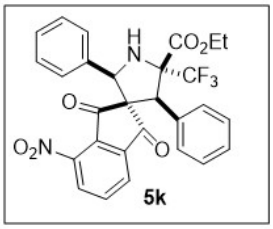


5j: The reaction was performed according to the general procedure 2, with imine **3a** (0.1 mmol, 25.9 mg) and arylidene-indandione **6j** (0.2 mmol, 50.4 mg). The product occurs as yellow crystals with a melting range of 180.9-184.1 °C, an isolated yield of 40% and a dr of 50:50:0:0:0.

R_f: 0.75 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{28}H_{20}F_4NO_4$: 512.1479 $[M+H]^+$; found: 512.1484.

^{1}H-NMR (700 MHz, $CDCl_3$, 298 K): δ = 7.56-7.50 (m, 3H), 7.35-7.34 (m, 1H), 7.22-7.20 (m, 1H), 7.16-7.10 (m, 21H), 4.91-4.85 (m, 4H), 4.64/4.61 (2s, 2H), 4.29-4.23 (m, 2H), 3.96-3.89 (m, 2H), 0.95 (2t, J = 7.2 Hz, 6H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.26 (s, 3F), -74.33 (s, 3F), -110.56 - -110.60 (m, 1F), -111.35 - -111.39 (m, 1H) ppm; ^{13}C-NMR (176 MHz, $CDCl_3$, 298 K): δ = 198.4, 198.4, 166.7, 166.5, 158.4, 158.1, 156.9, 156.6, 143.9, 143.7, 138.0, 138.0, 137.8, 137.7, 133.3, 133.3, 133.2, 133.2, 130.3, 130.3, 129.0, 128.8, 128.8, 128.7, 126.7, 125.8 (q, J = 283 Hz), 123.5, 123.4, 123.1, 123.0, 119.0, 119.0, 119.0, 74.5 (q, J = 30 Hz), 72.7, 72.6, 71.8, 71.6, 63.1, 60.7, 60.6, 13.4, 13.4 ppm (mixture of 2 diastereomers).

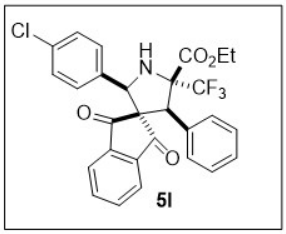


5k: The reaction was performed according to the general procedure 2, with imine **3a** (0.1 mmol, 25.9 mg) and arylidene-indandione **6a** (0.2 mmol, 55.8 mg). The product occurs as yellow oil with an isolated yield of 46% and a dr of 60:40:0:0:0.

R_f: 0.66 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{28}H_{20}F_3N_2O_6$: 539.1424 $[M+H]^+$; found: 539.1427.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 7.98-7.95 (m, 1H), 7.89-7.86 (m, 1H), 7.82-7.79 (m, 1H), 7.75-7.72 (m, 2H), 7.67-7.65 (m, 1H), 7.16-7.10 (m, 20H), 4.98-4.84 (m, 4H), 4.69, 4.63 (2s, 2H), 4.32-4.22 (m, 2H), 3.99-3.87 (m, 2H), 0.96 (2t, J = 7.1 Hz, 6H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.33 (s, 3F), -74.35 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 197.1, 196.7, 193.5, 193.2, 166.7, 166.3, 144.4, 143.4, 143.0, 136.4, 136.2, 133.1, 132.8, 130.3, 129.8, 129.5, 129.0, 128.8, 128.7, 128.6, 128.6, 128.6, 128.5, 127.8 (q, J = 281 Hz), 126.7, 126.5, 126.4, 74.3 (q, J = 30 Hz), 73.3, 72.5, 72.4, 72.0, 63.2, 61.1, 60.2, 13.3 ppm (mixture of 2 diastereomers).

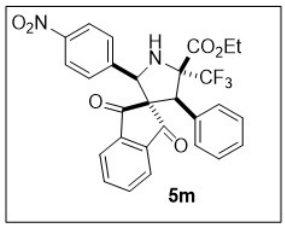


5l: The reaction was performed according to the general procedure 2, with imine **3l** (0.1 mmol, 29.4 mg) and arylidene-indandione **6a** (0.2 mmol, 46.8 mg). The product occurs as yellow oil with an isolated yield of 69% and a dr of 100:0:0:0.

R_f: 0.65 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{28}H_{20}ClF_3NO_4$: 528.1184 $[M+H]^+$; found: 528.1188.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 7.77-7.74 (m, 1H), 7.65-7.58 (m, 3H), 7.10-7.04 (m, 9H), 4.90-4.78 (m, 2H), 4.61 (s, 1H), 4.30-4.19 (m, 1H), 3.95-3.84 (m, 1H), 0.93 (t, J = 7.2 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.21 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.4, 199.3, 166.7, 142.6, 142.0, 136.2, 135.9, 135.9, 134.3, 133.3, 132.3, 130.1, 128.7, 128.4, 128.4, 128.3, 128.1, 125.8 (q, J = 298 Hz), 123.1, 123.1, 74.6 (q, J = 28 Hz), 71.7, 70.3, 63.1, 61.0, 13.3 ppm.

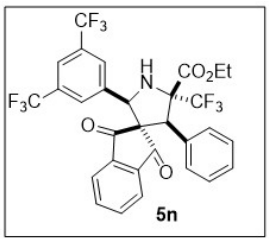


5m: The reaction was performed according to the general procedure 2, with imine **3m** (0.1 mmol, 30.5 mg) and arylidene-indandione **6a** (0.2 mmol, 46.8 mg). The product occurs as yellow oil with an isolated yield of 74% and a dr of 100:0:0:0.

R_f: 0.58 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{28}H_{20}F_3N_2O_6$: 539.1424 $[M+H]^+$; found: 539.1428.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 8.00-7.97 (m, 2H), 7.80-7.78 (m, 1H), 7.67-7.56 (m, 3H), 7.33-7.30 (m, 2H), 7.13-7.06 (m, 5H), 5.04-4.88 (m, 2H), 4.63 (s, 1H), 4.30-4.19 (m, 1H), 3.94-3.83 (m, 1H), 0.92 (t, J = 7.1 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.17 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.2, 199.1, 166.5, 147.7, 142.5, 141.8, 141.3, 136.5, 136.2, 132.8, 130.0, 128.6, 127.7, 126.2 (q, J = 298 Hz), 123.6, 123.3, 123.2, 74.6 (q, J = 28 Hz), 71.5, 69.6, 63.3, 61.6, 32.0, 29.2, 22.8, 14.3, 13.3 ppm.



5n: The reaction was performed according to the general procedure 2, with imine **3n** (0.1 mmol, 25.9 mg) and arylidene-indandione **6a** (0.2 mmol, 39.6 mg). The product occurs as yellow oil with an isolated yield of 31% and a dr of 100:0:0:0.

R_f: 0.75 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{30}H_{19}F_9NO_4$: 630.1321 $[M+H]^+$; found: 630.1321.

^{1}H-NMR (300 MHz, $CDCl_3$, 298 K): δ = 7.83-7.81 (m, 1H), 7.69-7.57 (m, 4H), 7.55-7.52 (m, 2H), 7.14-7.09 (m, 5H), 5.04-4.86 (m, 2H), 4.65 (s, 1H), 4.30-4.19 (m, 1H), 3.93-3.83 (m, 1H), 0.93 (t, J = 7.1 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -63.18 (s, 6H), -74.15 (s, 3F) ppm; ^{13}C-NMR (75 MHz, $CDCl_3$, 298 K): δ = 199.1, 198.9, 166.4, 142.5, 141.8, 136.9, 136.5, 136.2, 135.8, 132.8, 131.8 (q, J = 34 Hz), 130.0, 129.6 (q, J = 270 Hz), 128.5, 126.8, 123.4, 123.3, 123.1 (q, J = 271 Hz), 122.3, 121.1, 74.4 (J = 28 Hz), 71.4, 69.4, 63.4, 61.2, 54.7, 13.3 ppm.

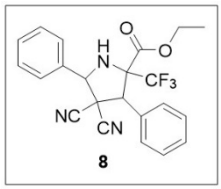
3.3 Formal (3+2)-Cycloaddition – Benzylidene-Malonitrile

3a
1 eq.

7
2 eq.

8

General procedure 3: To a stirred solution of benzylidene-malonitrile **7** (0.2 mmol, 30.8 mg) in dry DCM (2 mL), LiOH (3 eq., 7.2 mg), TEBAC (30 mol%, 7.8 mg) and imine **3a** (0.1 mmol, 25.9 mg) were added successively. The reaction mixture was stirred for 24 h at room temperature. The mixture was filtered over a pad of silica and washed with Et_2O. After evaporation of the solvent the product was purified by column chromatography with a gradient of heptane and ethylacetate (20:1 – 10:1 – 5:1) to yield product **8** with yield and diastereomeric ratio stated below.



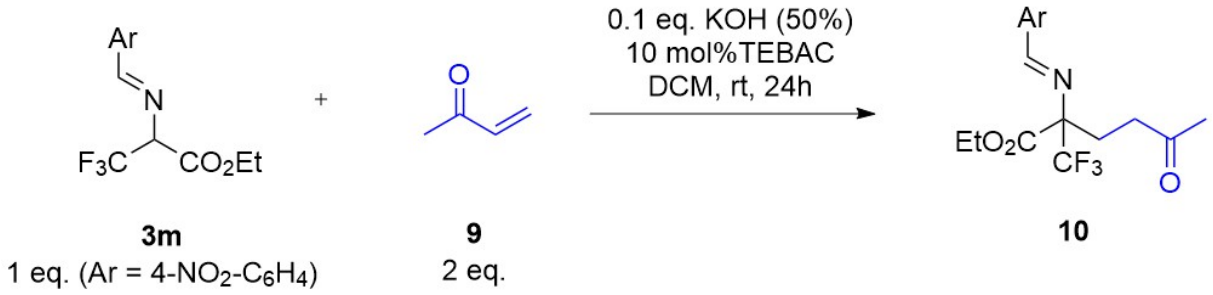
8: The reaction was performed according to the general procedure 3. The product occurs as white oil with an isolated yield of 60% (mixture of the two main diastereomers) and a dr of 49:33:16:2.

R_f: 0.82 (Heptane/EtOAc: 1/1).

HRMS (ESI): *m/z* calculated for $C_{22}H_{18}F_3N_3O_2$: 414.1424 $[M+H]^+$; found: 414.1423.

^{1}H-NMR (500 MHz, $CDCl_3$, 298 K): δ = 7.76-7.74 (m, 2H), 7.50-7.46 (m, 6H), 7.31-7.29 (m, 2H), 5.32 (d, J = 4.11 Hz, 1H), 4.49 (s, 1H), 3.96-3.89 (m, 1H), 3.58-3.51 (m, 1H), 3.40 (d, J = 4.11 Hz, 1H), 0.76 (t, J = 7.2 Hz, 3H) ppm; ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -74.03 (s, 3F) ppm; ^{13}C-NMR (125 MHz, $CDCl_3$, 298 K): δ = 167.6, 134.8, 133.8, 133.2, 130.9, 130.6, 130.1, 129.5, 129.3, 129.2, 127. 6, 124.0 (q, J = 287.2 Hz), 113.2, 112.1, 74.7 (q, J = 30.4 Hz), 70.4, 63.8, 57.8, 48.7, 13.2 ppm (main diastereomer).

3.4 Michael Addition – Methyl-Vinyl-Ketone

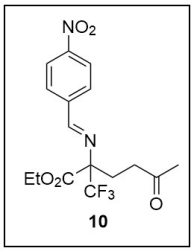


3m
1 eq. (Ar = 4-NO_2-C_6H_4)

9
2 eq.

10

General procedure 4: To a stirred solution of methyl-vinyl-ketone **9** (0.2 mmol, 16.7 µL) in dry DCM (2 mL), TEBAC (10 mol%, 2.6 mg), imine **3m** (0.1 mmol, 30.4 mg) and aq. KOH (50%, 0.1 eq., 1.2 µL) were added successively. The reaction mixture was stirred for 24 h at room temperature. The mixture was filtered over a pad of Na_2SO_4 and washed with Et_2O. After evaporation of the solvent the product was purified by column chromatography with a gradient of heptane and ethylacetate (2:1 – 1:1) to yield product **10** with 60% isolated yield.



10: The reaction was performed according to the general procedure 4. The product occurs as white oil with an isolated yield of 60%.

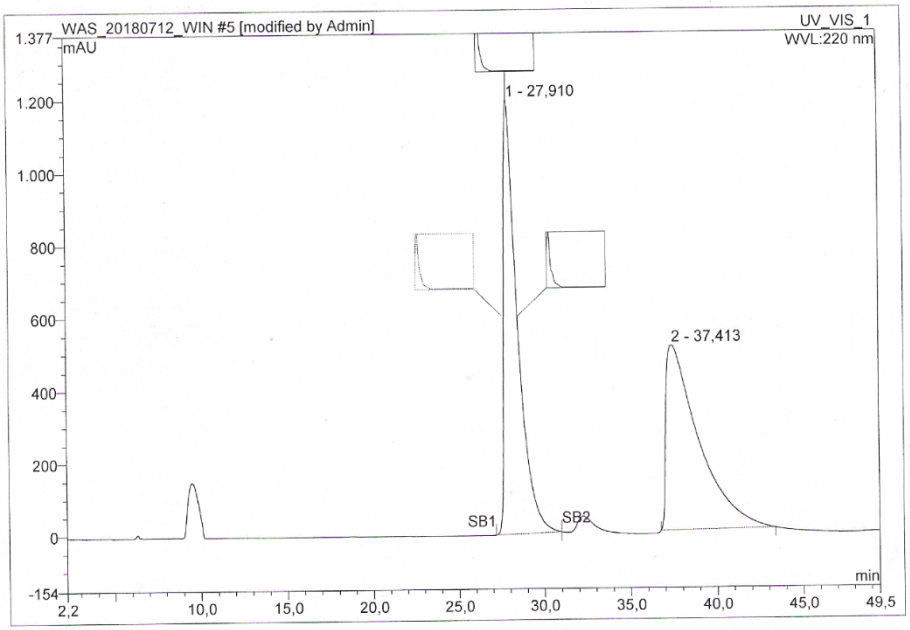
HRMS (ESI): *m/z* calculated for $C_{16}H_{17}F_3N_2O_5$: 375.1162 $[M+H]^+$; found: 375.1164.

^{1}H-NMR (500 MHz, $CDCl_3$, 298 K): δ = 8.51 (s, 1H), 8.31-8.29 (m, 2H), 7.98-7.97 (m, 2H), 4.33 (q, J = 7.1 Hz, 2H), 2.63-2.60 (m, 2H), 2.50-2.46 (m, 2H), 2.15 (s, 3H), 1.33 (t, J = 7.1 Hz, 3H); ^{19}F-NMR (282 MHz, $CDCl_3$, 298 K): δ = -71.90 (s, 3F) ppm; ^{13}C-NMR (125 MHz, $CDCl_3$, 298 K): δ = 206.5, 163.6, 163.3, 149.9, 140.7, 130.6, 129.7, 124.4 (q, J = 286.7 Hz), 124.1, 73.6 (q, J = 25.2), 63.0, 37.8, 30.2, 27.9, 14.1 ppm.

4. Copies of HPLC Chromatograms

5 WIN-432-02_99_1_flo5

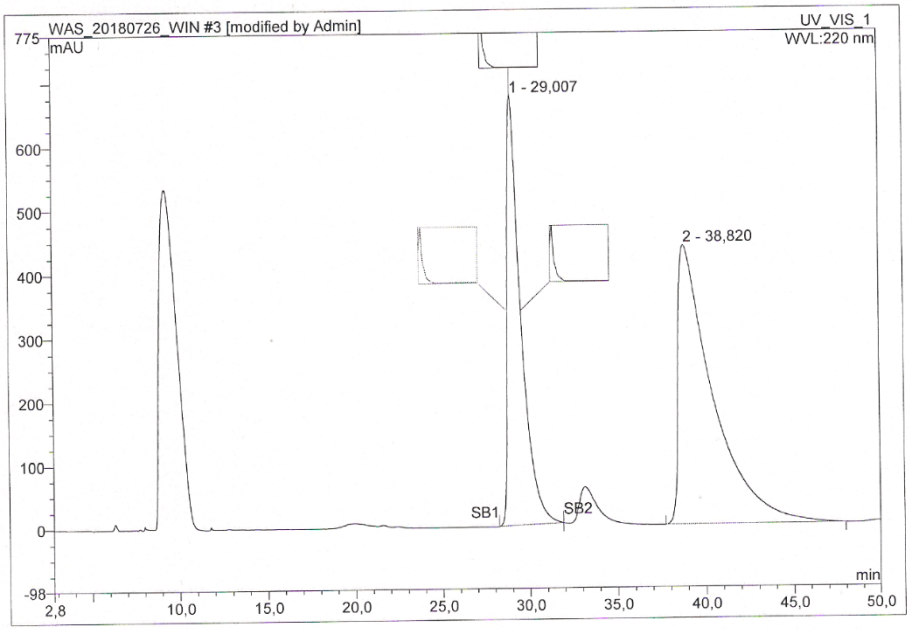
Sample Name:	**WIN-432-02_99_1_flo5**	*Injection Volume:*	**20,0**
Vial Number:	**RA3**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**220**
Control Program:	**AD_H_60Min_100A_flow0_5**	*Bandwidth:*	**4**
Quantif. Method:	**default**	*Temperature/Column:*	**10**
Recording Time:	**12.7.2018 14:40**	*Flow ml/min:*	**0,500**
Run Time (min):	**60,00**	*Sample Amount:*	**1,0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	27,91	n.a.	1196,866	1113,383	50,04	n.a.	BMB*
2	37,41	n.a.	508,798	1111,527	49,96	n.a.	BMB*
Total:			1705,664	2224,911	100,00	0,000	

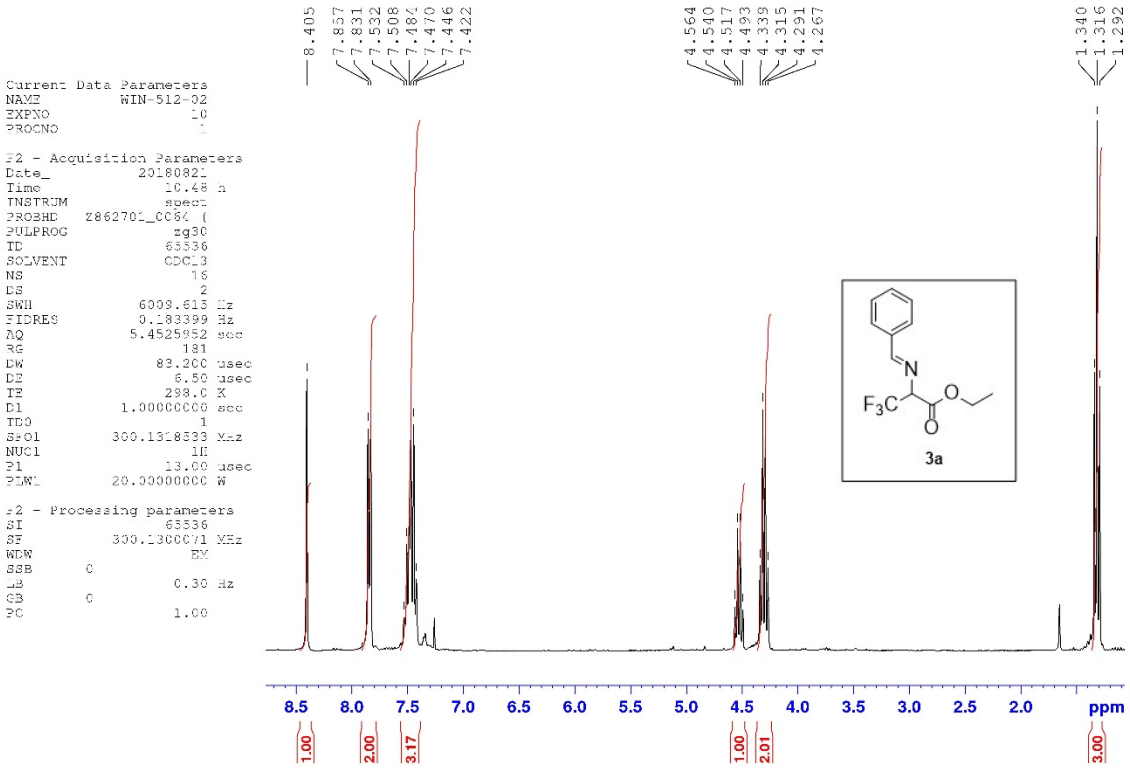
3 WIN-469-02_99_1_flo5

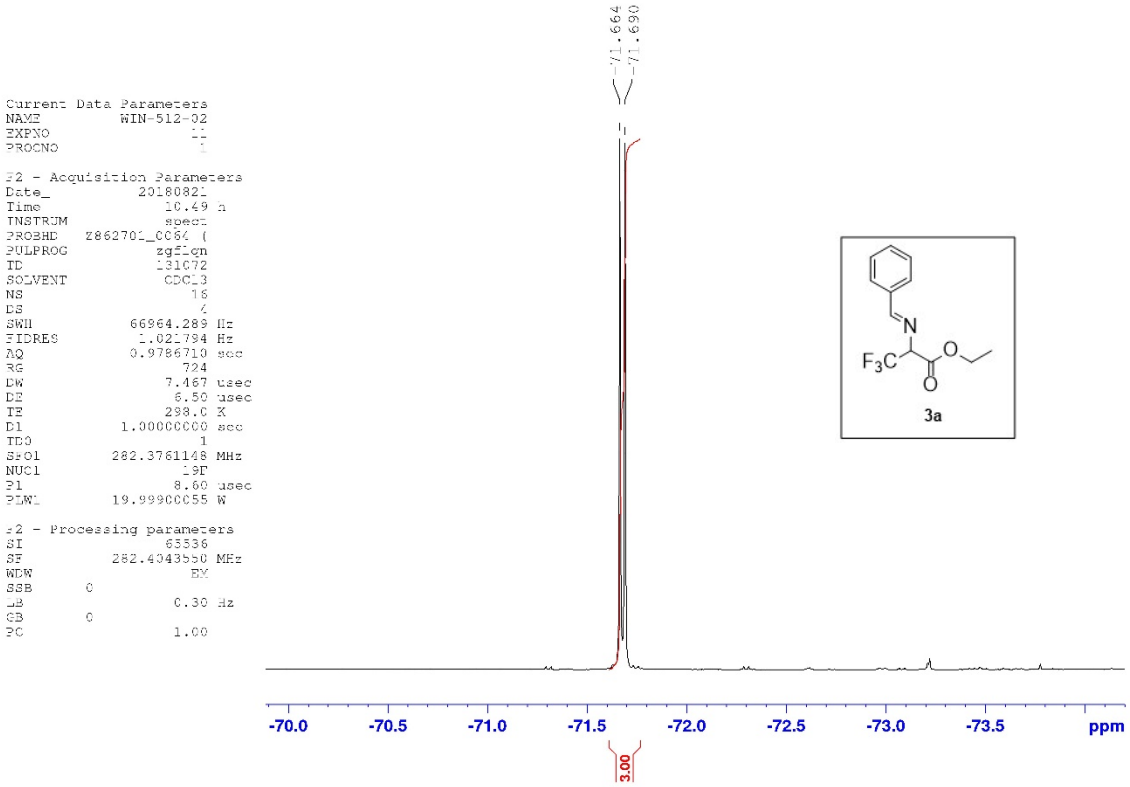
Sample Name:	**WIN-469-02_99_1_flo5**	*Injection Volume:*	**20,0**
Vial Number:	**RE2**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**220**
Control Program:	**AD_H_70Min_100A_flow0_5**	*Bandwidth:*	**4**
Quantif. Method:	**default**	*Temperature/Column:*	**10**
Recording Time:	**26.7.2018 12:16**	*Flow ml/min:*	**0,500**
Run Time (min):	**70,00**	*Sample Amount:*	**1,0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	29,01	n.a.	675,427	614,643	38,27	n.a.	BMB*
2	38,82	n.a.	437,777	991,465	61,73	n.a.	BMB*
Total:			1113,204	1606,108	100,00	0,000	

5. Copies of NMR-Spectra of new Compounds

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PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 724
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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-71.690
3a
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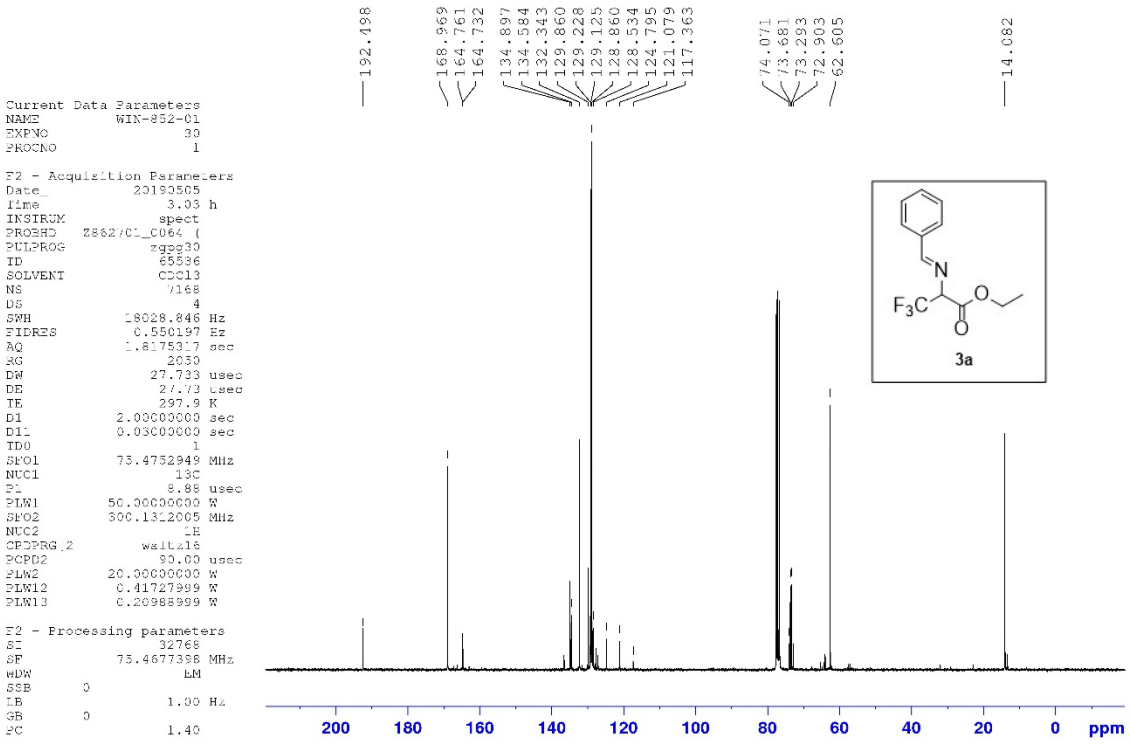
-70.5
-71.0
-71.5
-72.0
-72.5
-73.0
-73.5
ppm
3.00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PROCNO 1
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7168
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
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SF 75.4677398 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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164.761
164.732
134.897
134.584
132.343
129.860
129.228
129.125
128.860
128.534
124.795
121.079
117.363
74.071
73.681
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62.605
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140
120
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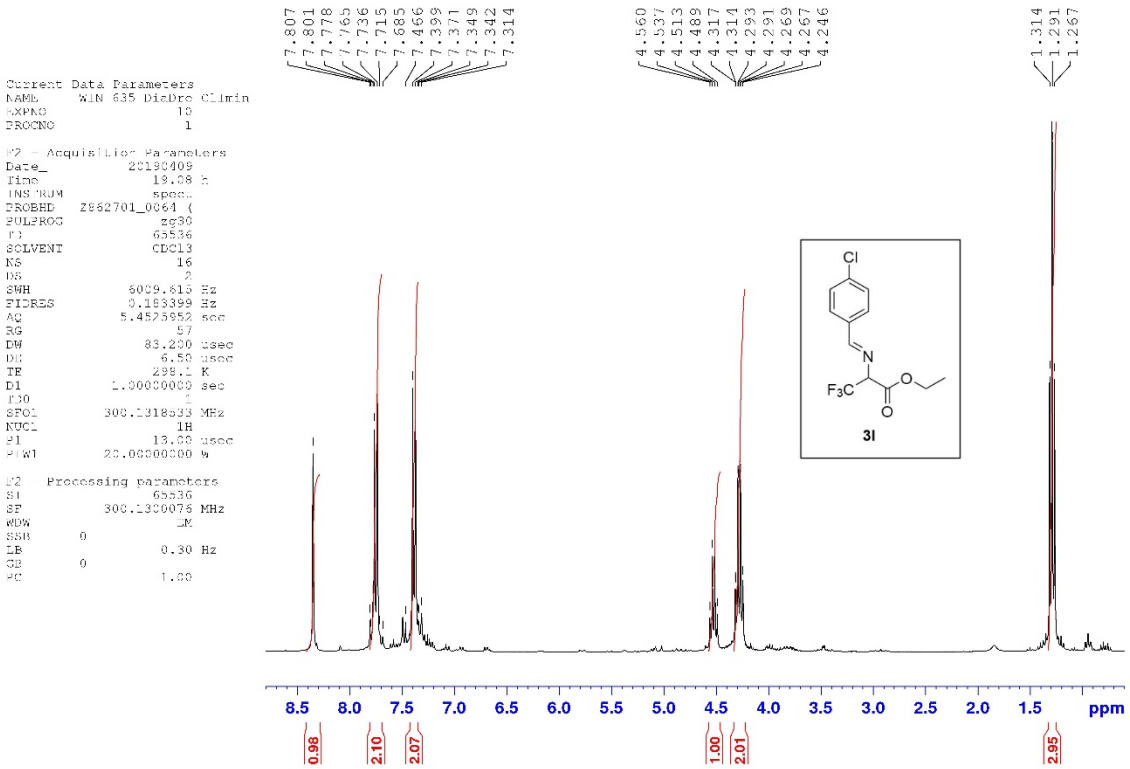
60
40
20
0
ppm

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PROCNO                  1

F2 - Acquisition Parameters
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PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.183399 Hz
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RG                    57
DW                83.200 usec
DE                 6.50 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1
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NUC1                  1H
P1                 13.00 usec
PLW1         20.00000000 W

F2 - Processing parameters
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SF           300.1300076 MHz
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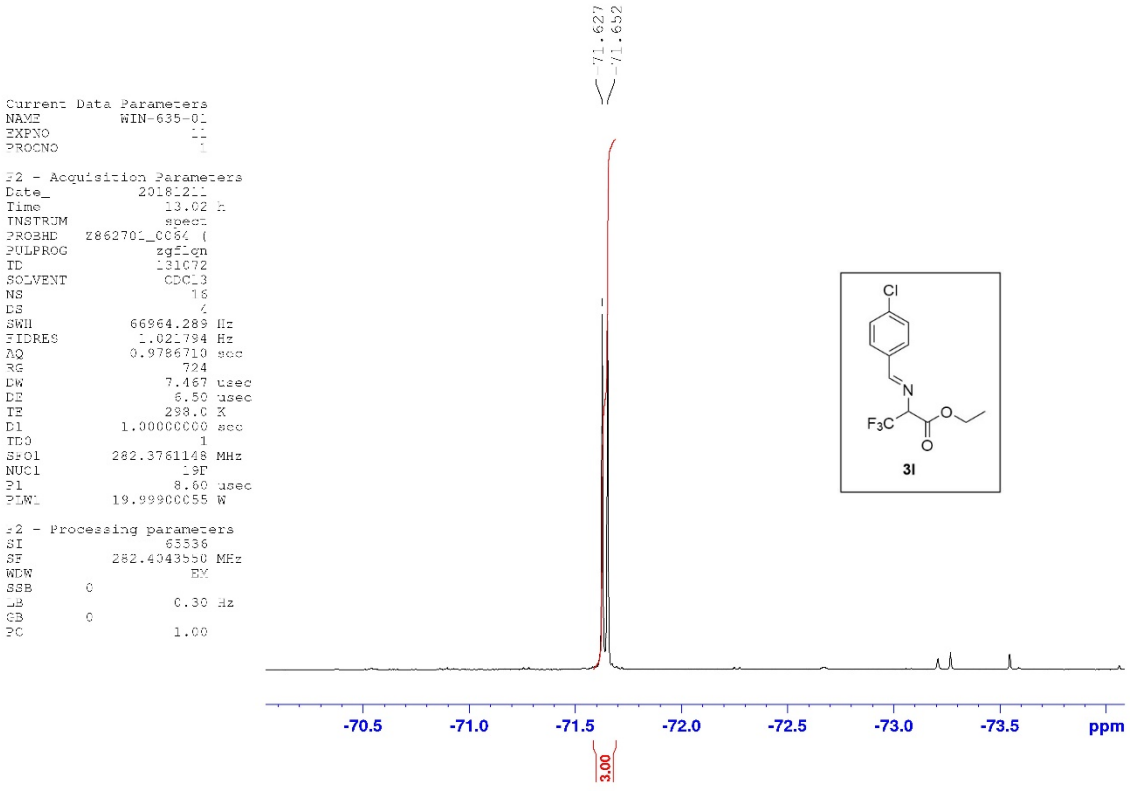


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PROCNO                 1

F2 - Acquisition Parameters
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TD                131072
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            66964.289 Hz
FIDRES          1.021794 Hz
AQ              0.9786710 sec
RG                   724
DW                7.467 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
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P1                 8.60 usec
PLW1         19.99900055 W

F2 - Processing parameters
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WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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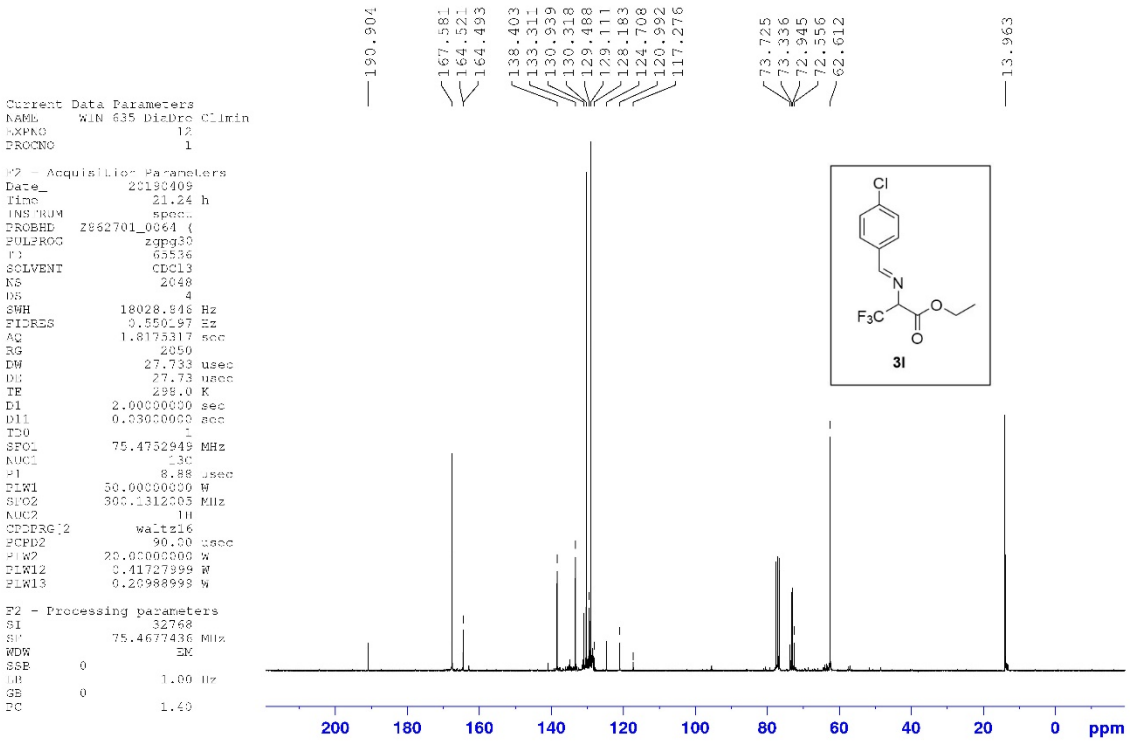


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EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
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PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
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FIDRES            0.550197 Hz
AQ            1.8175317 sec
RG                 2050
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NUC2                  1H
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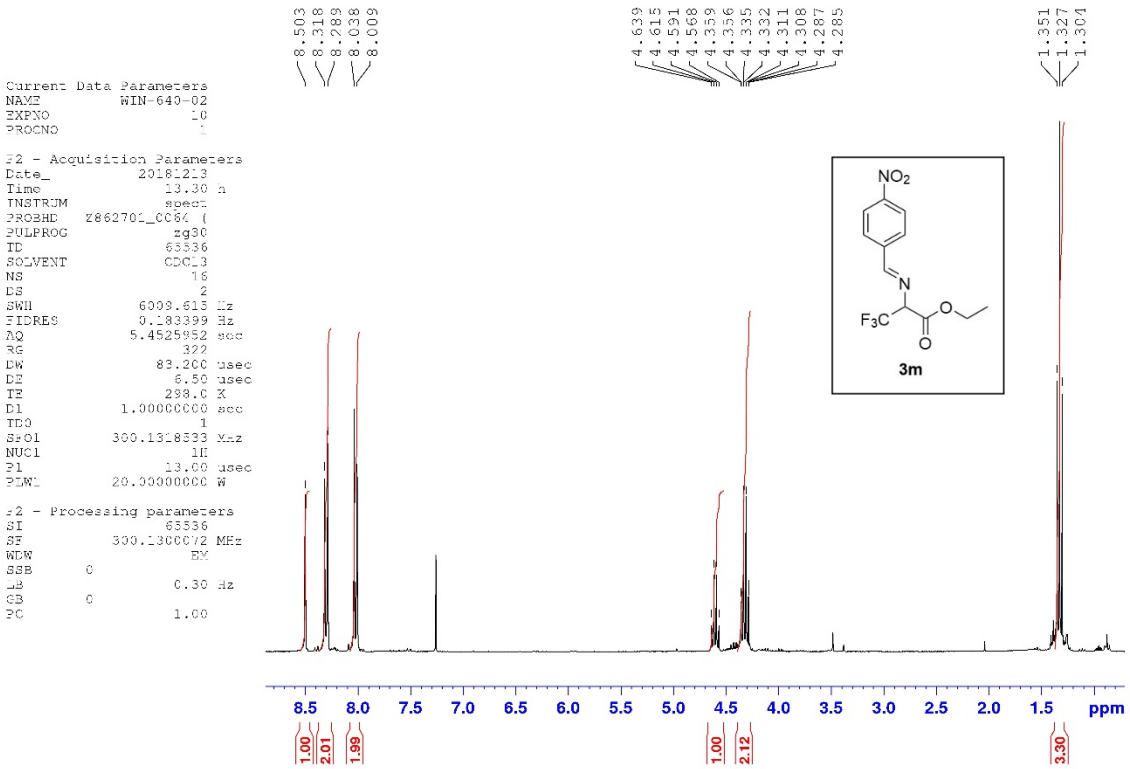


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PROCNO                 1

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INSTRUM             spect
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PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES            0.183399 Hz
AQ            5.4525952 sec
RG                  322
DW               83.200 usec
DE                6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         300.1318533 MHz
NUC1                  1H
P1                13.00 usec
PLW1         20.00000000 W

F2 - Processing parameters
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SF           300.1300072 MHz
WDW                   EM
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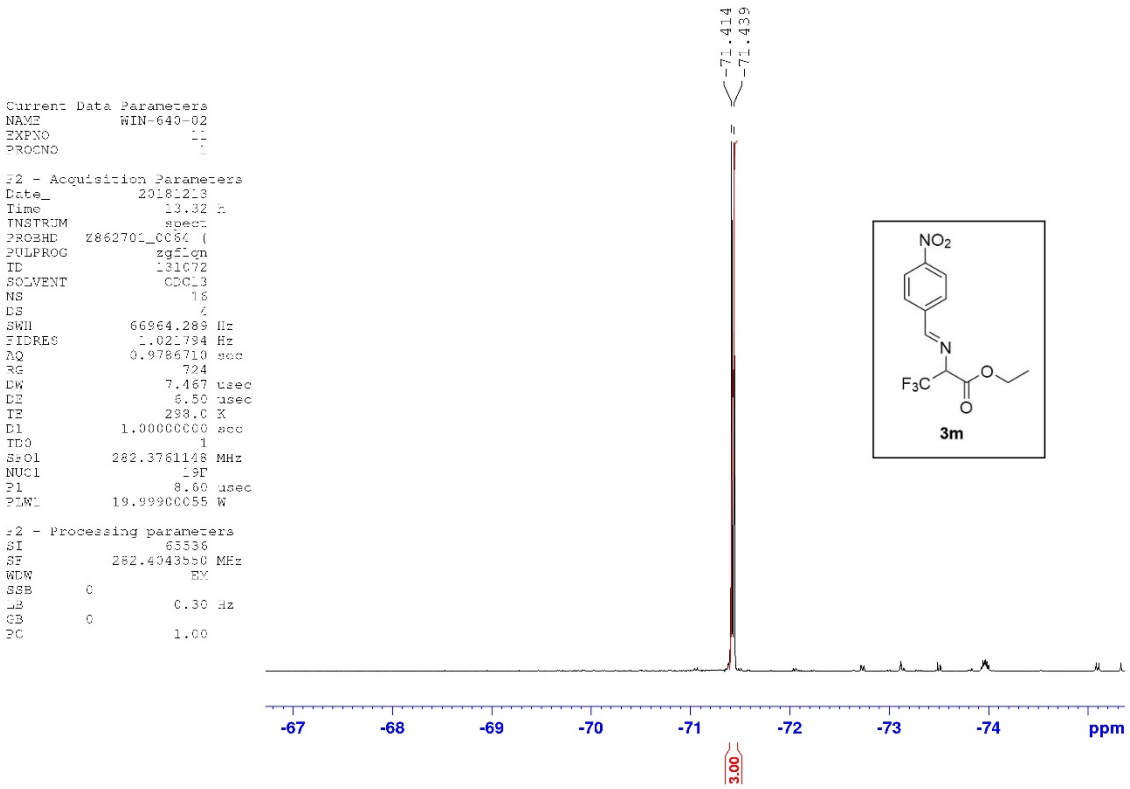

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PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 724
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W

F2 - Processing parameters
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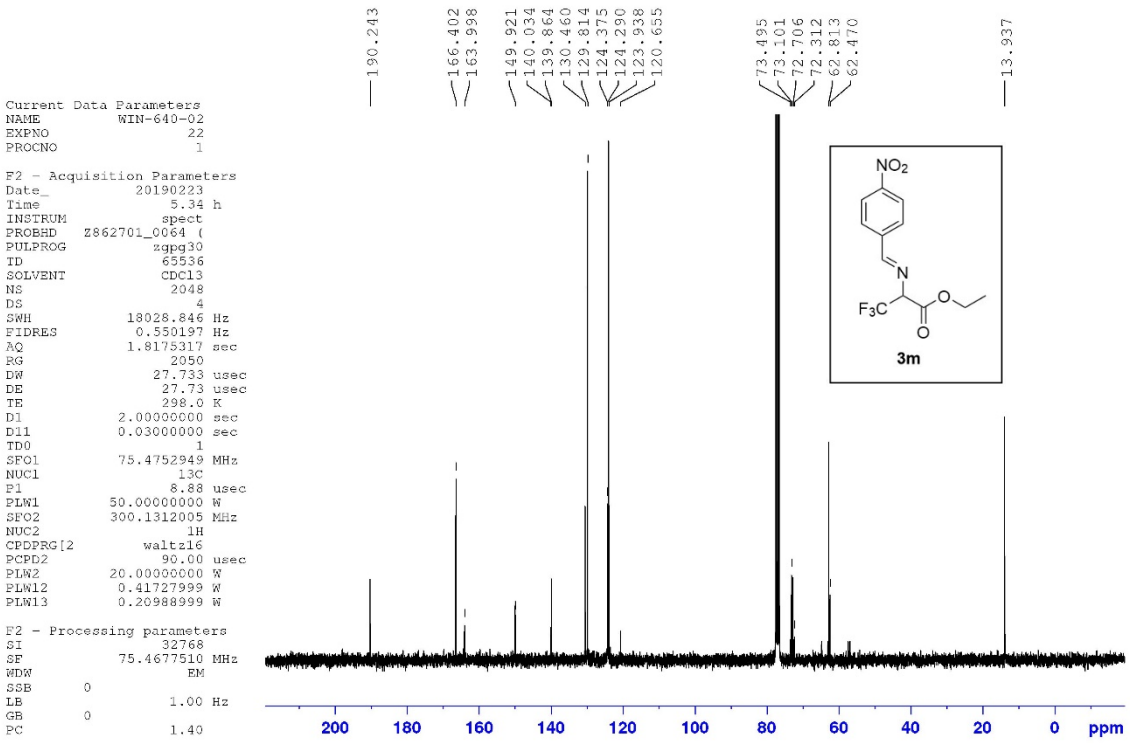
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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EXPNO 22
PROCNO 1

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Time 5.34 h
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TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
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F2 - Processing parameters
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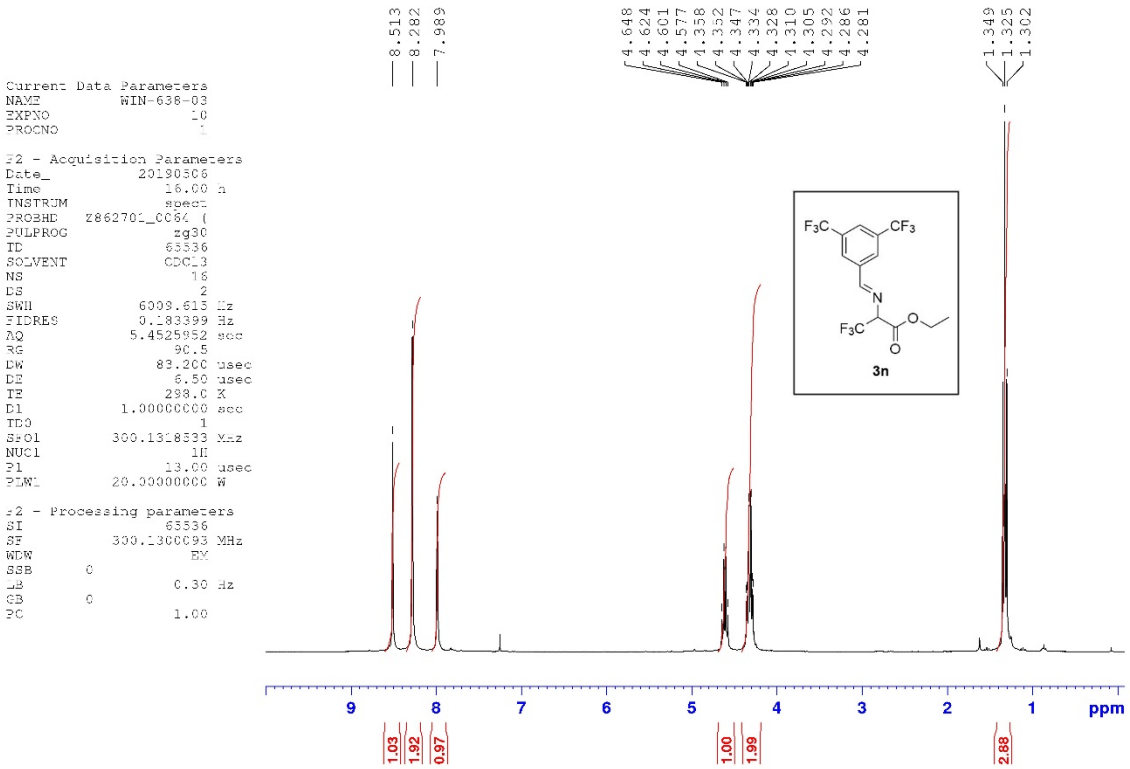


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PROCNO                 1

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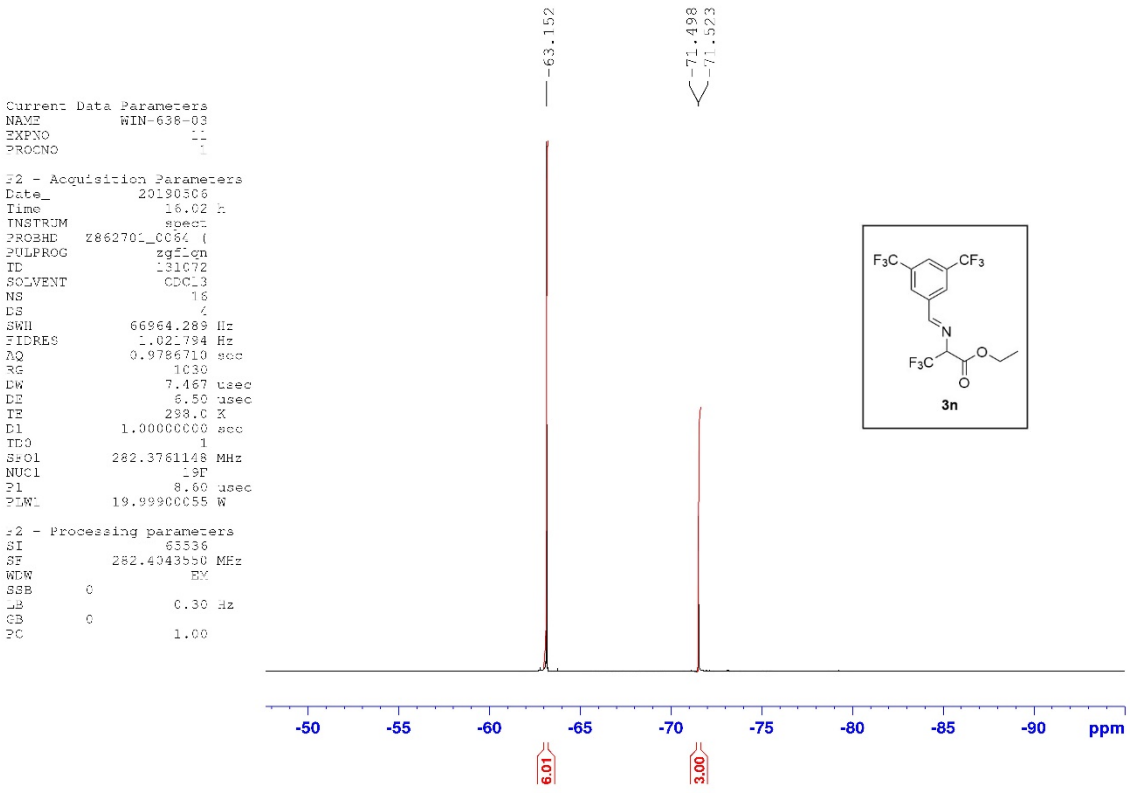
INSTRUM             spect
PROBHD    Z862701_CC84 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              5.4525952 sec
RG                  90.5
DW                 83.200 usec
DE                  6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1         300.1318533 MHz
NUC1                  1H
P1                 13.00 usec
PLW1         20.00000000 W

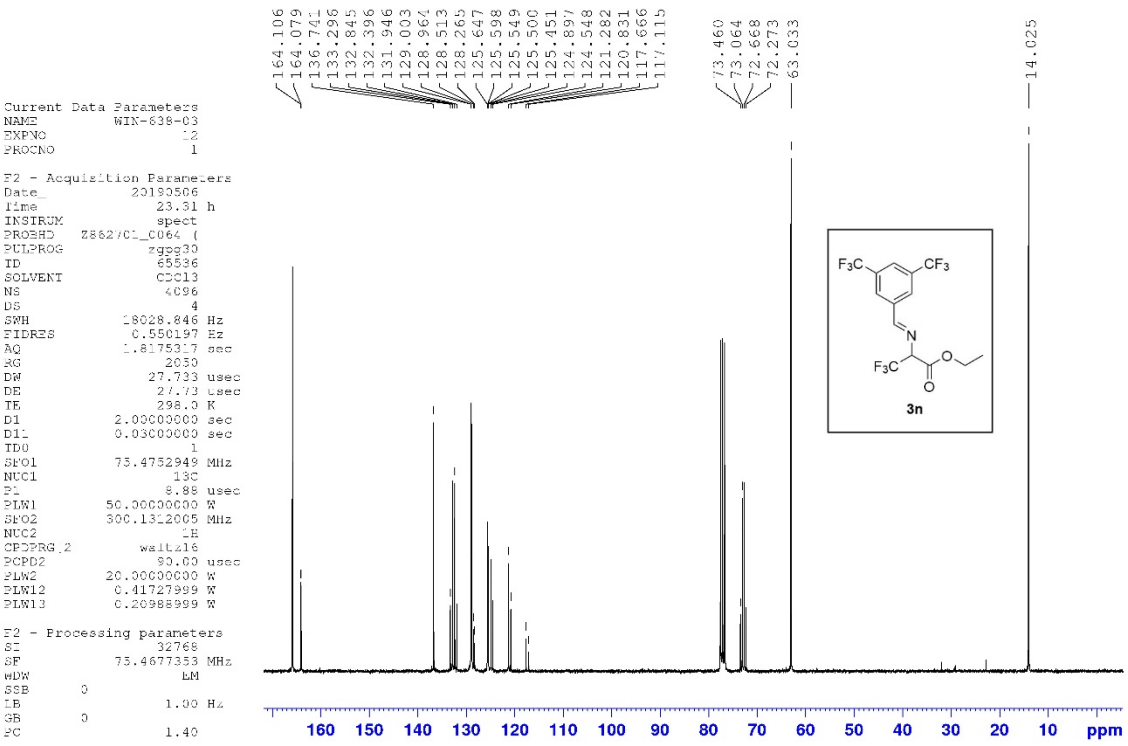
F2 - Processing parameters
SI                 65536
SF           300.1300093 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

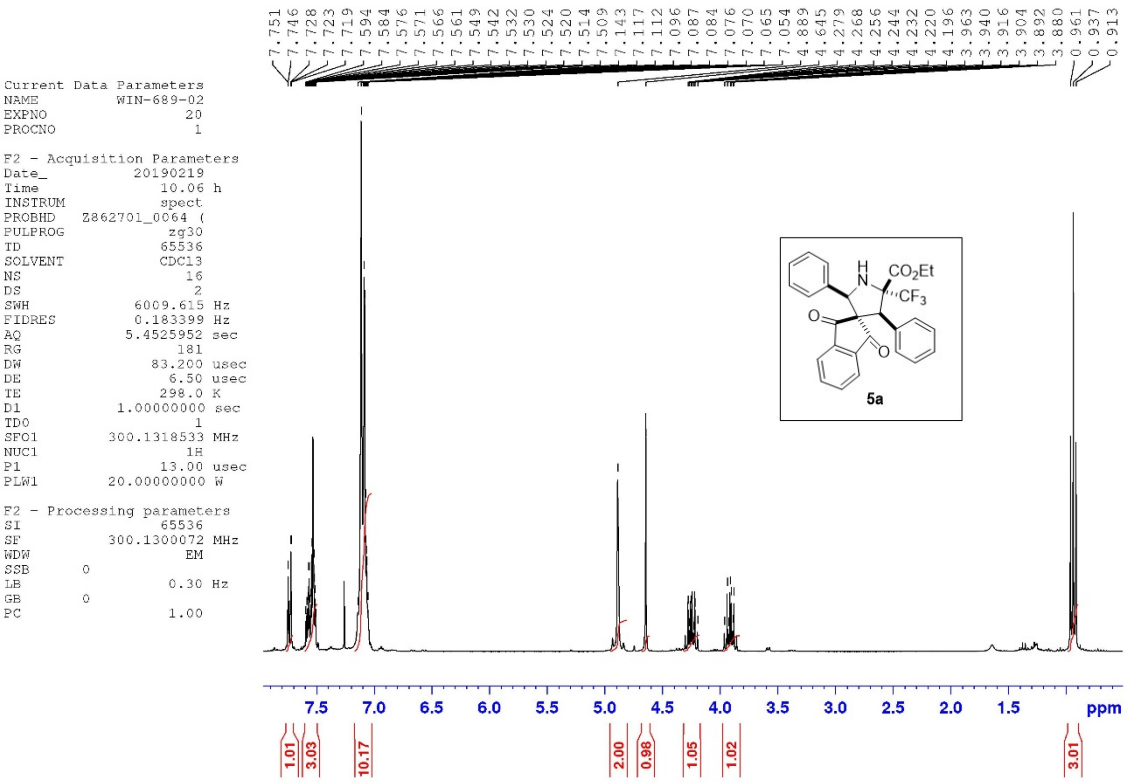



```
Current Data Parameters
NAME          WIN-638-03
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190506
Time              16.02 h
INSTRUM             spect
PROBHD    Z862701_CC84 (
PULPROG           zgflqn
TD                131072
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            66964.289 Hz
FIDRES          1.021794 Hz
AQ              0.9786710 sec
RG                  1030
DW                 7.467 usec
DE                  6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1         282.3761148 MHz
NUC1                  19F
P1                  8.60 usec
PLW1         19.99900055 W

F2 - Processing parameters
SI                 65536
SF           282.4043550 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

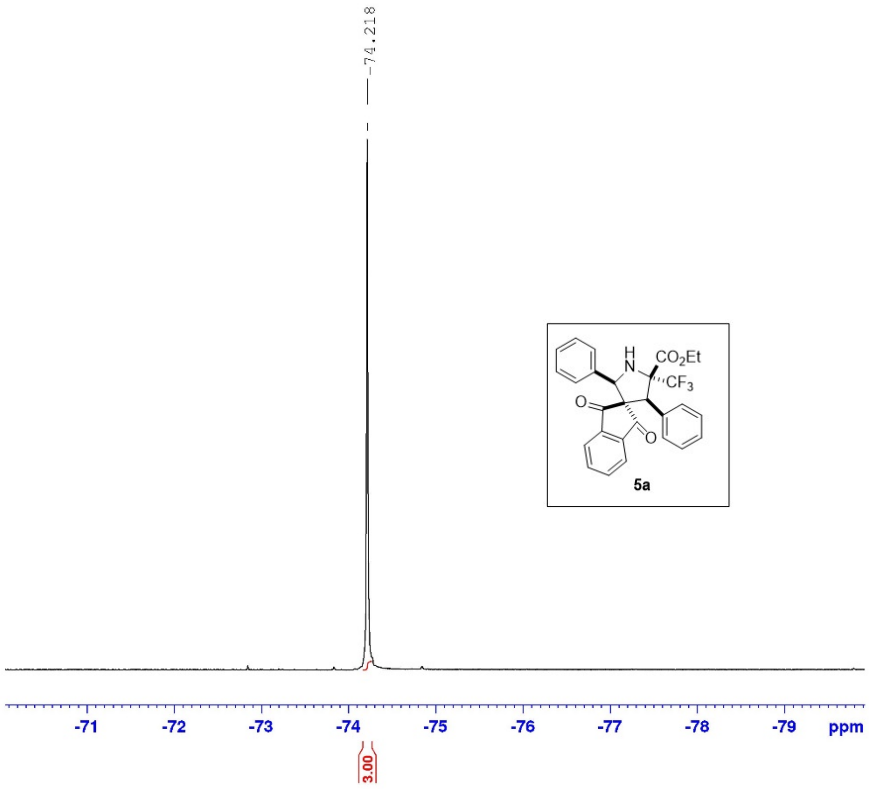

Current Data Parameters
NAME WIN-638-03
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190506
Time 23.31 h
INSTRUM spect
PROBHD Z862701_0064 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677353 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
164.106
164.079
136.741
133.296
132.845
132.396
131.946
129.003
128.964
128.513
128.265
125.647
125.598
125.549
125.500
125.451
124.897
124.548
121.282
120.831
117.666
117.115
73.460
73.064
72.668
72.273
63.033
14.025
F3C
CF3
N
F3C
O
O
3n
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Current Data Parameters
NAME WIN-689-02
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190219
Time 10.06 h
INSTRUM spect
PROBHD Z862701_0064 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 181
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.751
7.746
7.728
7.723
7.719
7.594
7.584
7.576
7.571
7.566
7.561
7.549
7.542
7.532
7.530
7.524
7.520
7.514
7.509
7.143
7.117
7.112
7.096
7.087
7.084
7.076
7.070
7.065
7.054
4.889
4.645
4.279
4.268
4.256
4.244
4.232
4.220
4.196
3.963
3.940
3.916
3.904
3.892
3.880
0.961
0.937
0.913
H
N
CO2Et
CF3
O
O
5a
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
1.01
3.03
10.17
2.00
0.98
1.05
1.02
3.01

```
Current Data Parameters
NAME          WIN-689-02
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190215
Time              13.56 h
INSTRUM             spect
PROBHD    Z862701_0064 (
PULPROG           zgflqn
TD                131072
SOLVENT             CDCl3
NS                    16
DS                     4
SWH            66964.289 Hz
FIDRES          1.021794 Hz
AQ              0.9786710 sec
RG                    645
DW                7.467 usec
DE                6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1         282.3761148 MHz
NUC1                 19F
P1                 8.60 usec
PLW1         19.99900055 W

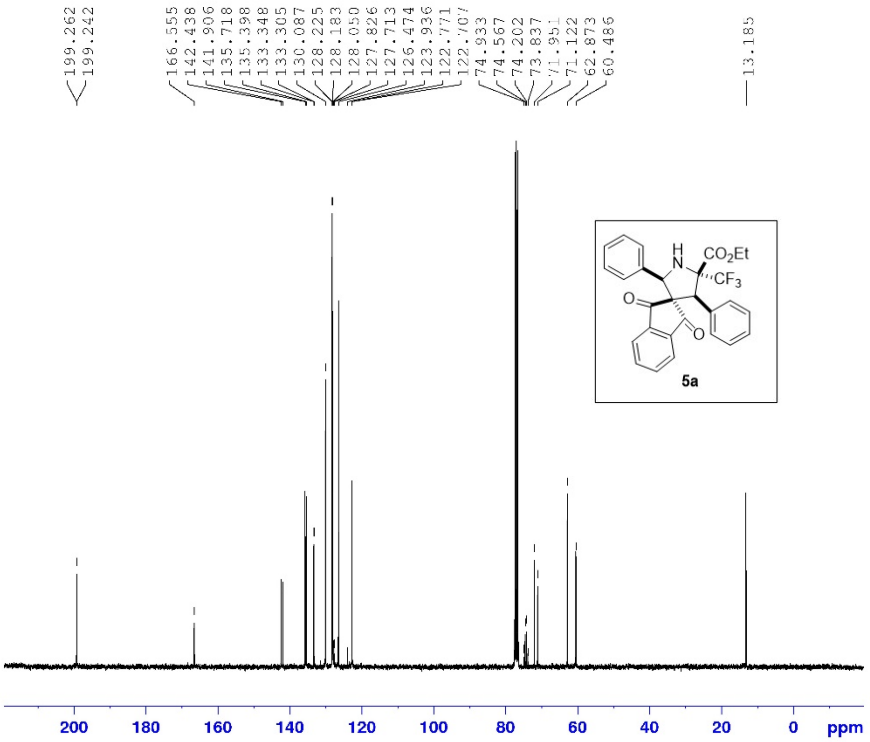
F2 - Processing parameters
SI                 65536
SF           282.4043550 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

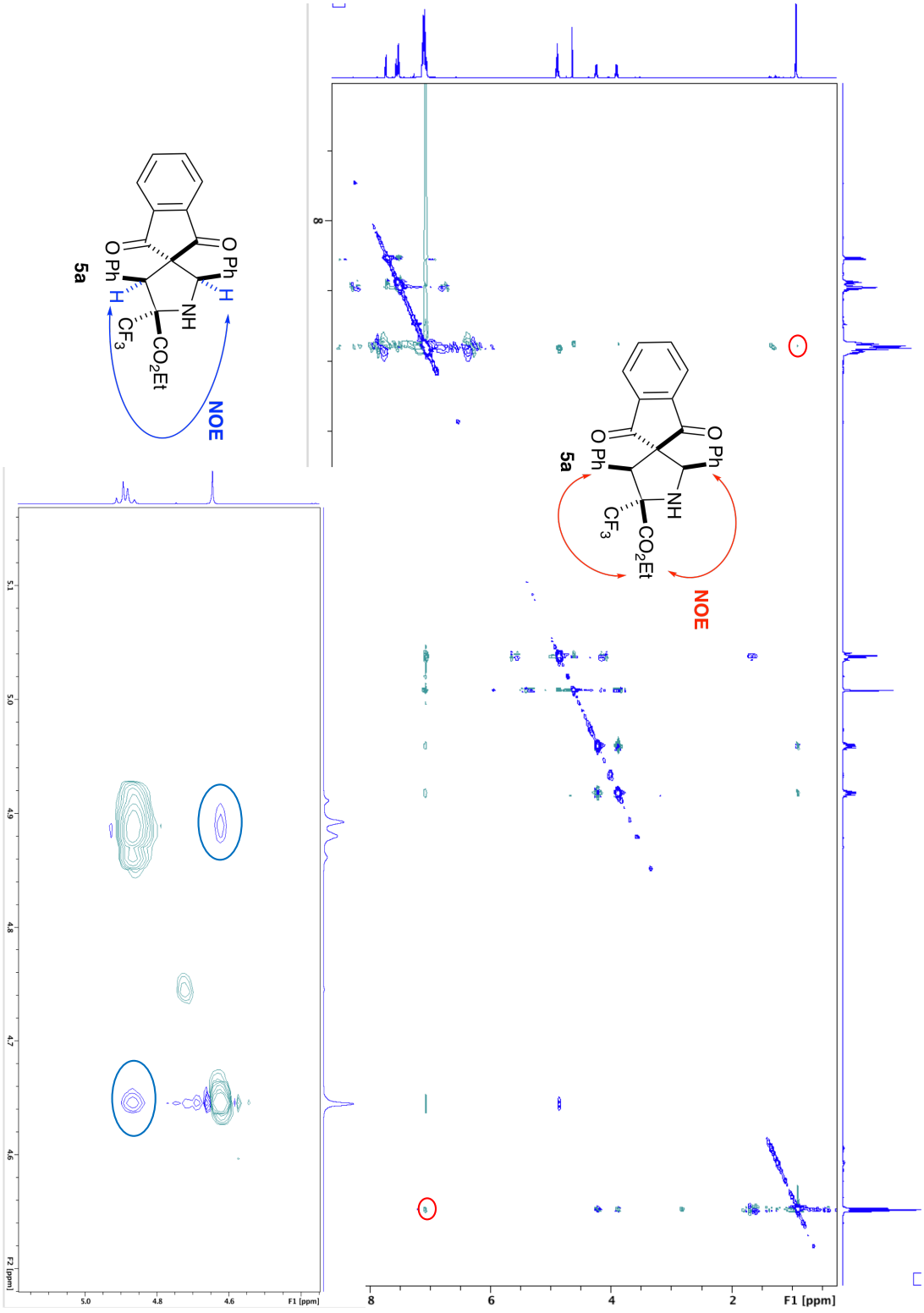


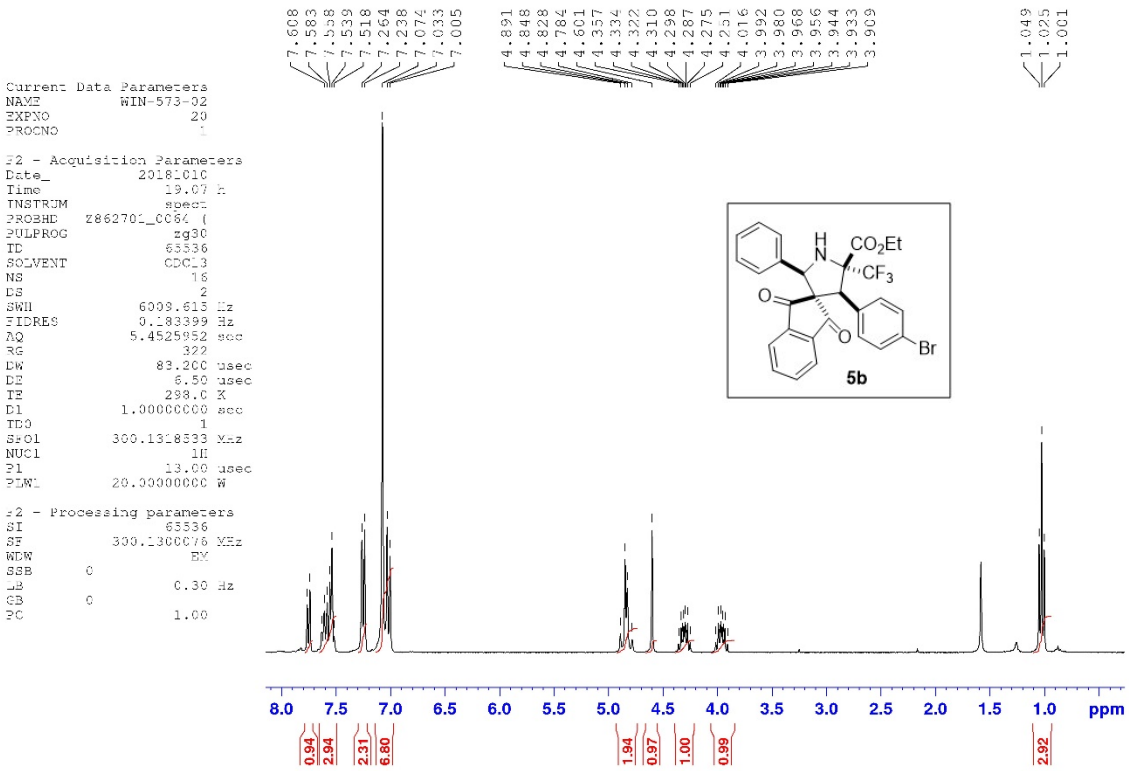

```
Current Data Parameters
NAME          WIN-689-02
EXPNO                 21
PROCNO                 1

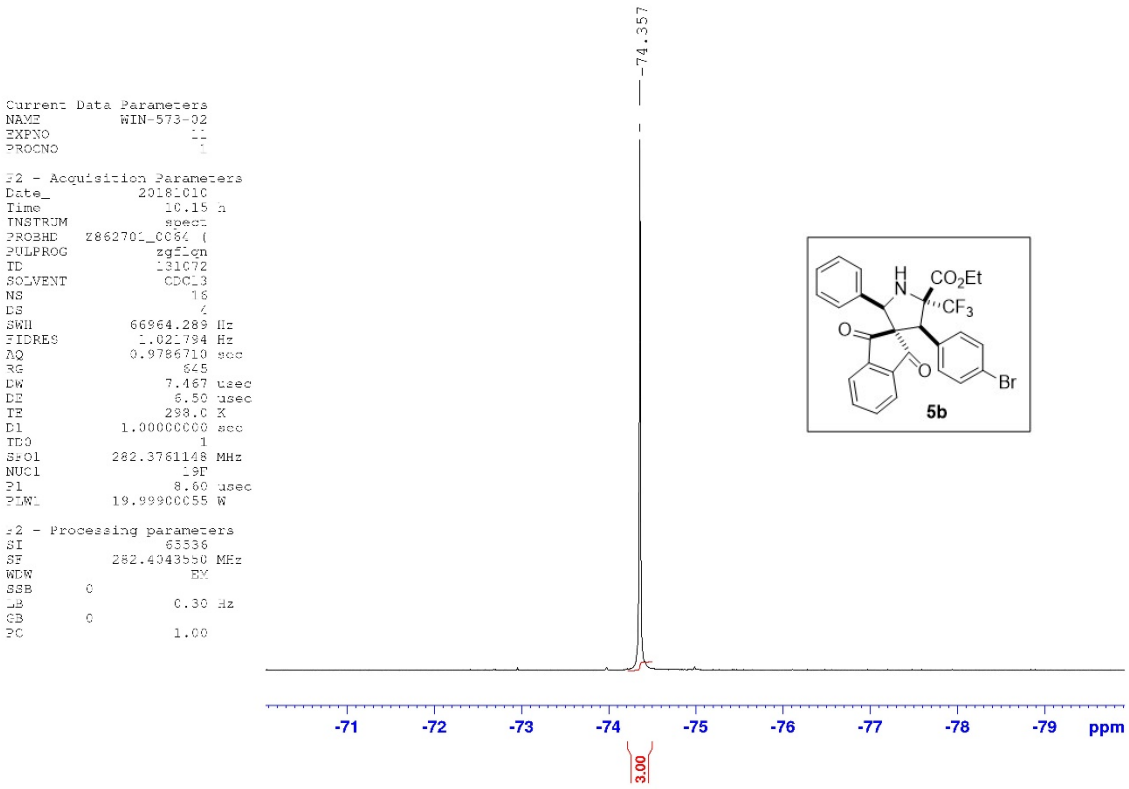
F2 - Acquisition Parameters
Date_           20190219
Time              21.27 h
INSTRUM             spect
PROBHD    Z862701_0064 (
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                  2048
DS                     4
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              1.8175317 sec
RG                  2050
DW               27.733 usec
DE                27.73 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         75.4752949 MHz
NUC1                 13C
P1                 8.88 usec
PLW1         50.00000000 W
SFO2        300.1312005 MHz
NUC2                 1H
CPDPRG_2        waltz16
PCPD2             90.00 usec
PLW2         20.00000000 W
PLW12         0.41727999 W
PLW13         0.20988999 W

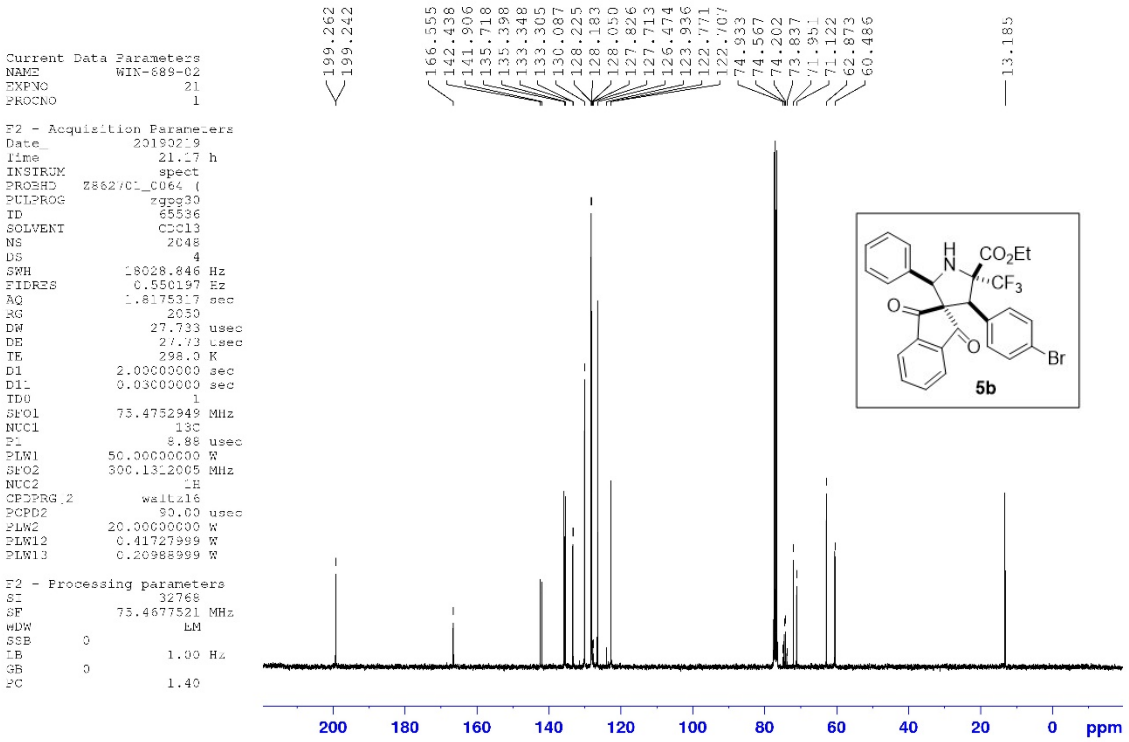
F2 - Processing parameters
SI                 32768
SF           75.4677521 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

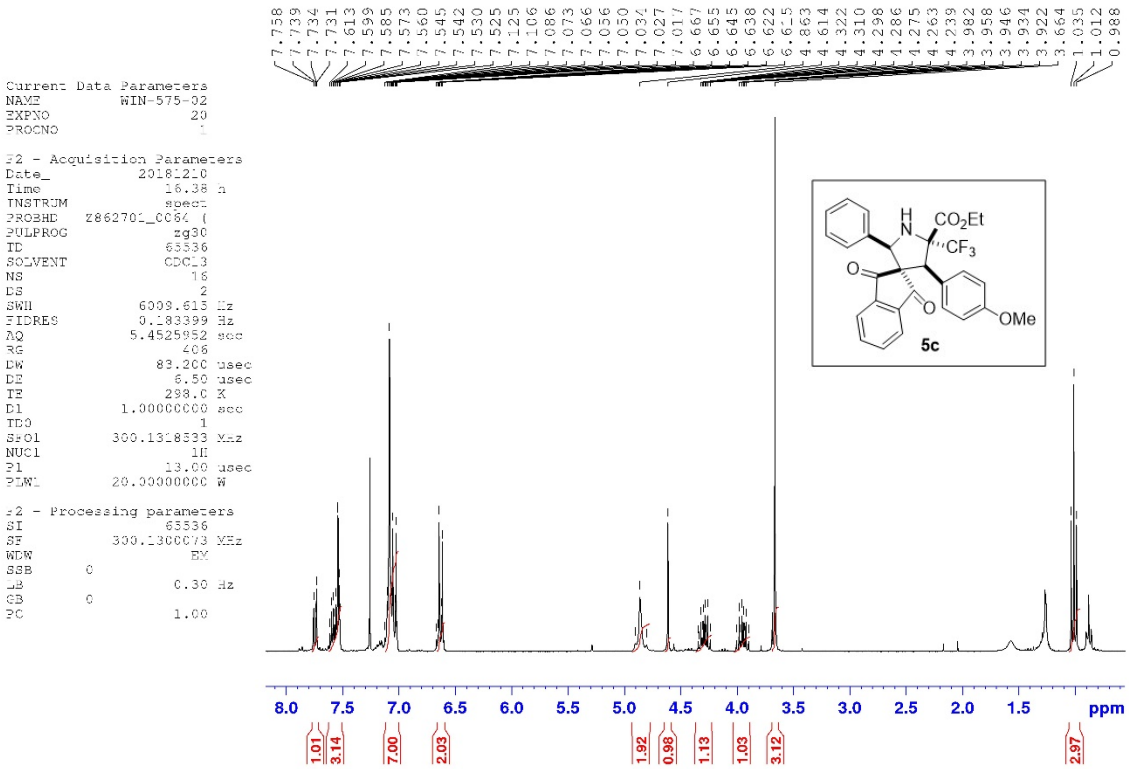


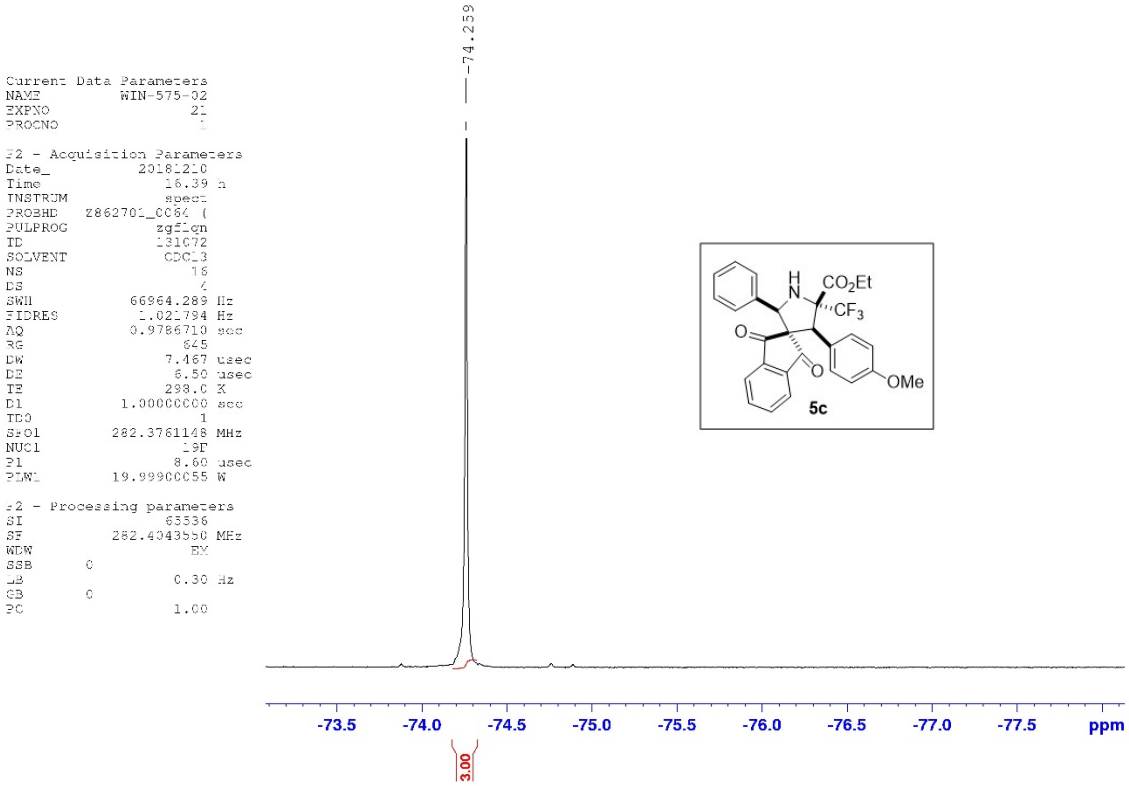

O
Ph
H
NH
CF3
CO2Et
5a
NOE
F1 [ppm]
F2 [ppm]


Current Data Parameters
NAME WIN-573-02
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181010
Time 19.07 h
INSTRUM spect
PROBHD Z862701_CC64 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 322
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318633 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.608
7.583
7.558
7.539
7.518
7.264
7.238
7.074
7.033
7.005
4.891
4.848
4.828
4.784
4.601
4.357
4.334
4.322
4.310
4.298
4.287
4.275
4.251
4.016
3.992
3.980
3.968
3.956
3.944
3.933
3.909
1.049
1.025
1.001
CO2Et
CF3
Br
5b
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.94
2.94
2.31
6.80
1.94
0.97
1.00
0.99
2.92


Current Data Parameters
NAME WIN-573-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181010
Time 10.15 h
INSTRUM spect
PROBHD Z862701_CC64 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 645
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-74.357
CO2Et
CF3
Br
5b
-71
-72
-73
-74
-75
-76
-77
-78
-79
ppm
3.00


Current Data Parameters
NAME WIN-689-02
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190219
Time 21.17 h
INSTRUM spect
PROBHD Z8827C1_C064 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2030
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677521 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
199.262
199.242
166.555
142.438
141.906
135.718
135.398
133.348
133.305
130.087
128.225
128.183
128.050
127.826
127.713
126.474
123.936
122.771
74.933
74.567
74.202
73.837
71.951
71.122
62.873
60.486
13.185
5b
200
180
160
140
120
100
80
60
40
20
0
ppm


Current Data Parameters
NAME WIN-575-02
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181210
Time 16.38 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 406
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.758
7.739
7.734
7.731
7.613
7.599
7.585
7.573
7.560
7.545
7.542
7.530
7.525
7.125
7.106
7.086
7.073
7.066
7.056
7.050
7.034
7.027
7.017
6.667
6.655
6.645
6.638
6.622
6.615
4.863
4.614
4.322
4.310
4.298
4.286
4.275
4.263
4.239
3.982
3.958
3.946
3.934
3.922
3.664
1.035
1.012
0.988
5c
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.01
3.14
7.00
2.03
1.92
0.98
1.13
1.03
3.12
2.97


Current Data Parameters
NAME WIN-575-02
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181210
Time 16.39 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 645
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-74.259
H
N
CO2Et
CF3
O
O
OMe
5c
-73.5
-74.0
-74.5
-75.0
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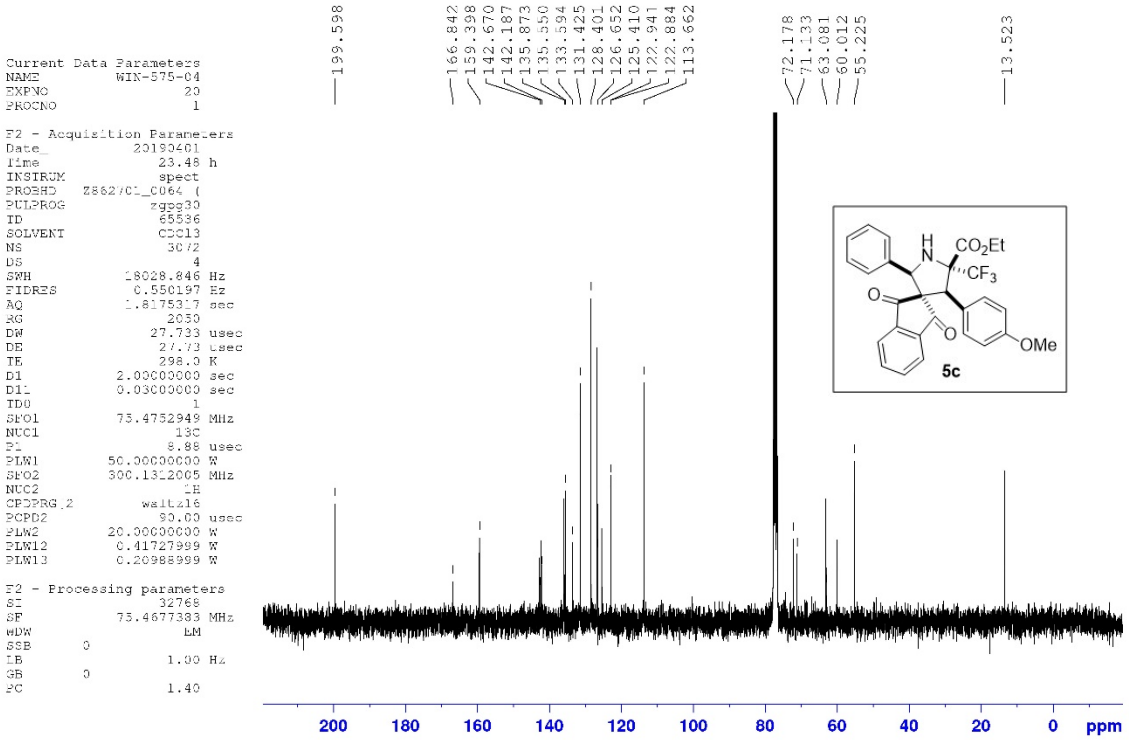
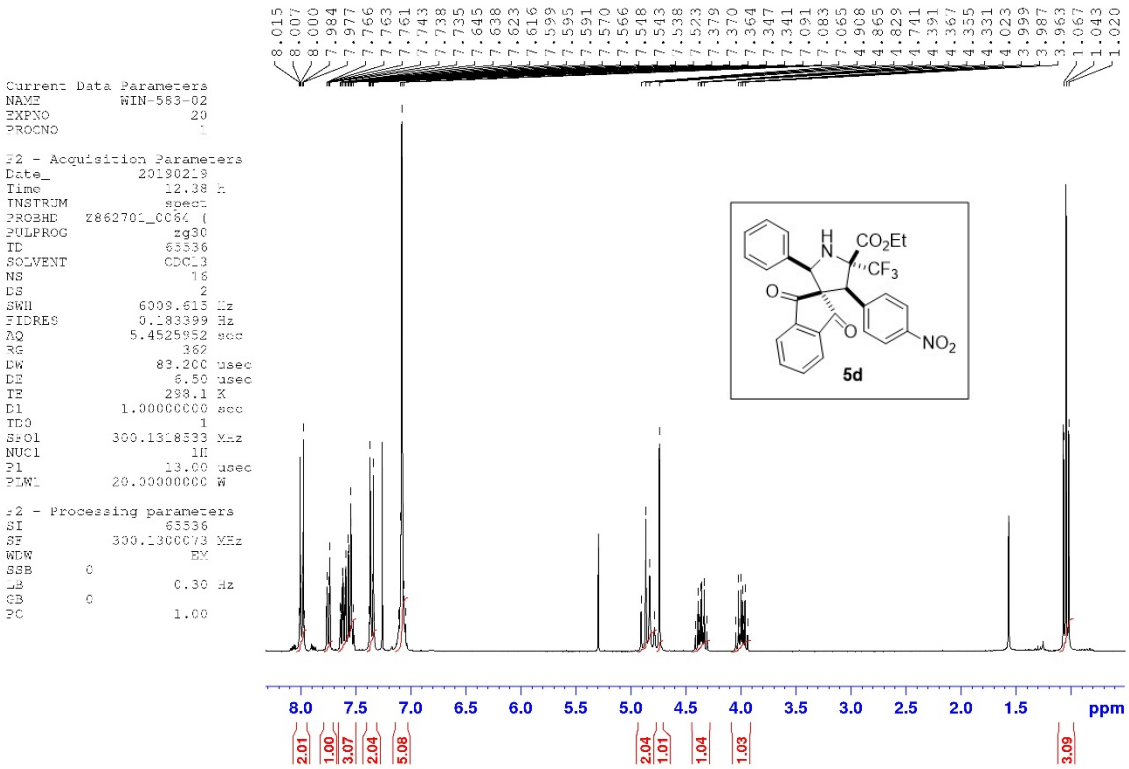
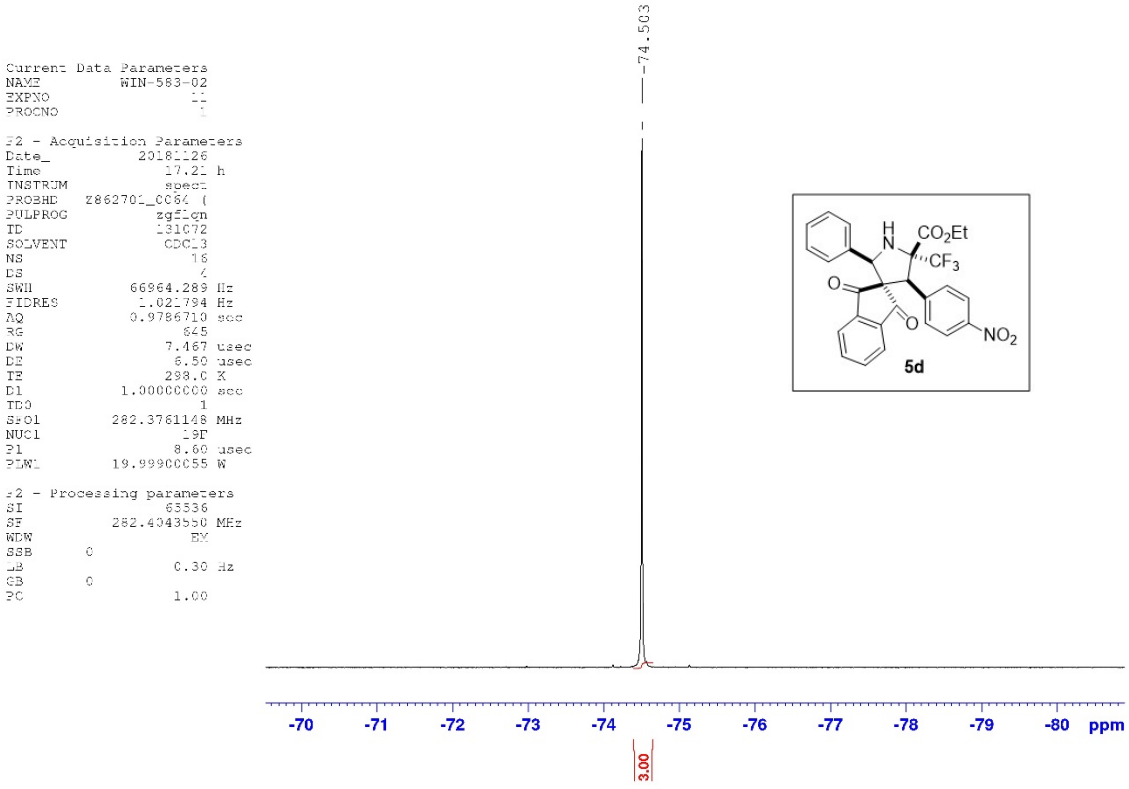
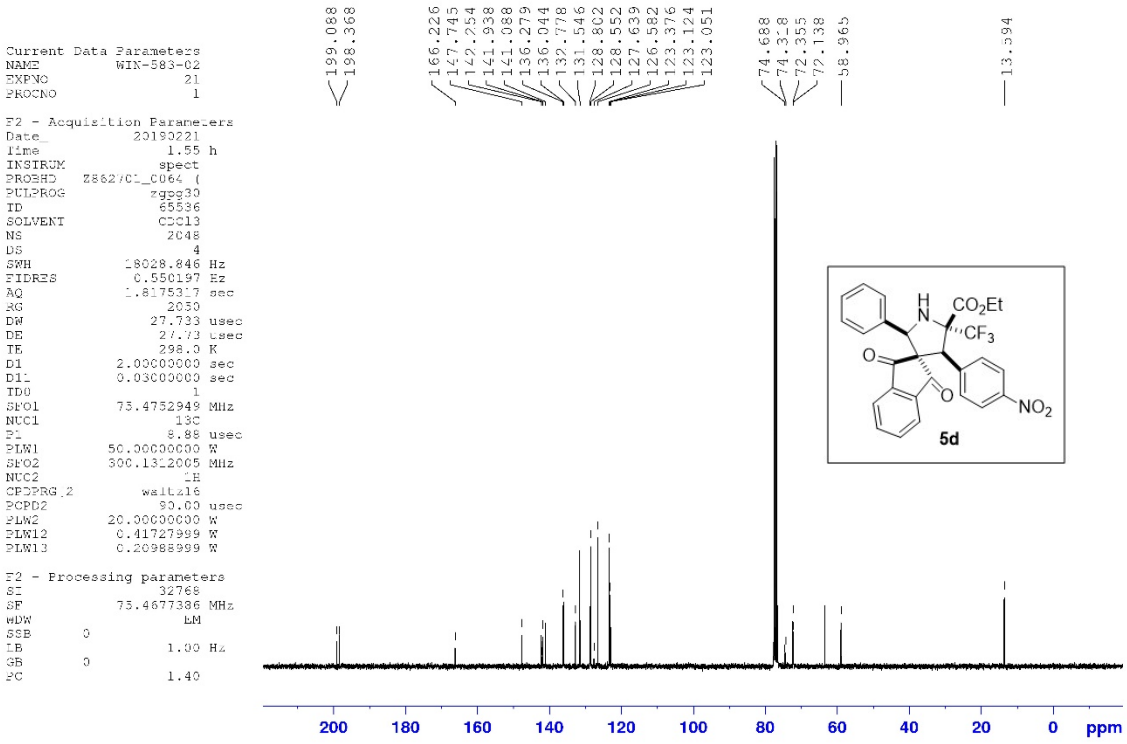
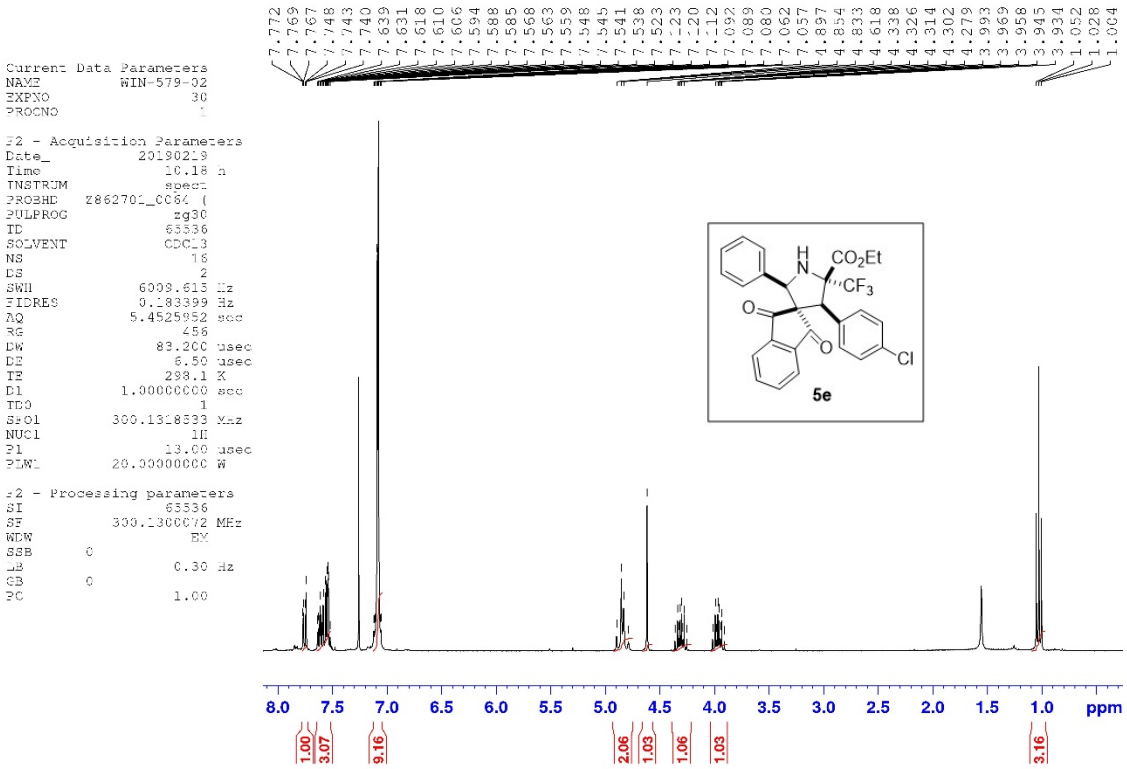
-76.5
-77.0
-77.5
ppm
3.00

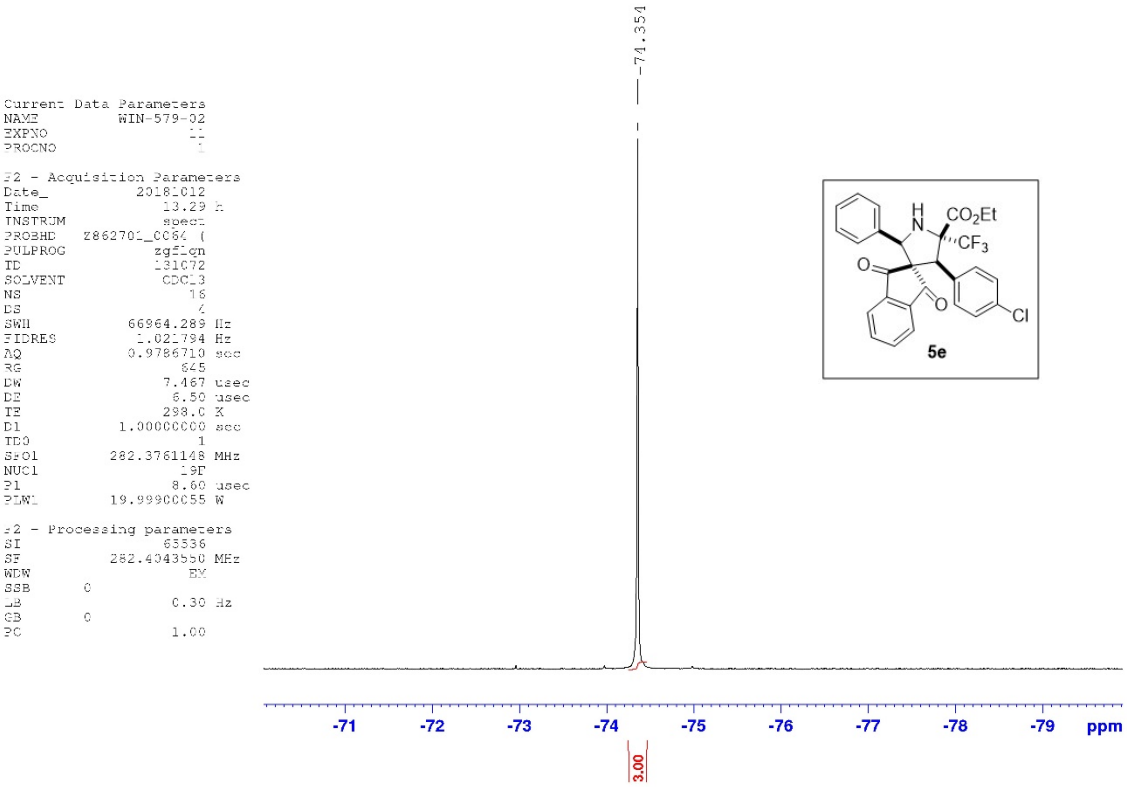

Current Data Parameters
NAME WIN-575-04
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190401
Time 23.48 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677383 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
199.598
166.842
159.398
142.670
142.187
135.873
135.550
133.594
131.425
128.401
126.652
125.410
122.941
122.884
113.662
72.178
71.133
63.081
60.012
55.225
13.523
H
N
CO2Et
CF3
O
O
OMe
5c
200
180
160
140
120
100
80
60
40
20
0
ppm

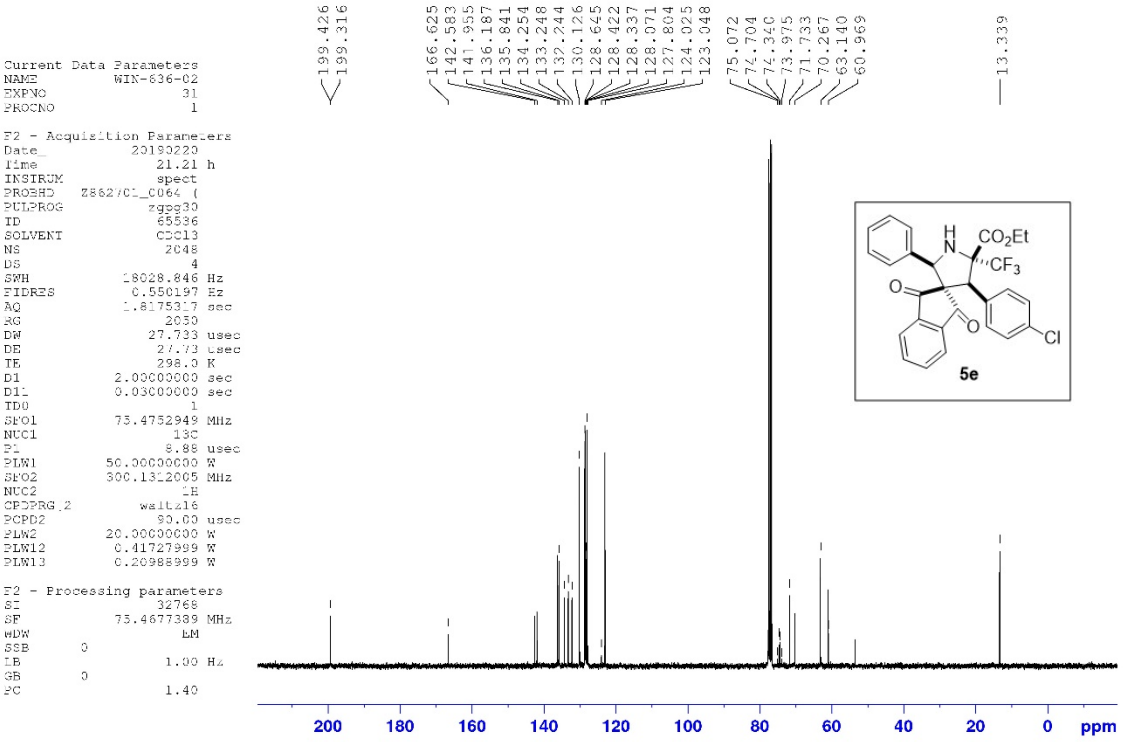

8.015
8.007
8.000
7.984
7.977
7.766
7.763
7.761
7.743
7.738
7.735
7.645
7.638
7.623
7.616
7.599
7.595
7.591
7.570
7.566
7.548
7.543
7.538
7.523
7.379
7.370
7.364
7.347
7.341
7.091
7.083
7.065
4.908
4.865
4.829
4.741
4.391
4.367
4.355
4.331
4.023
3.999
3.987
3.963
1.067
1.043
1.020
Current Data Parameters
NAME WIN-583-02
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190219
Time 12.38 h
INSTRUM spect
PROBHD Z862701_CC84 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 362
DW 83.200 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
H
N
CO2Et
CF3
O
O
NO2
5d
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
2.01
1.00
3.07
2.04
5.08
2.04
1.01
1.04
1.03
3.09

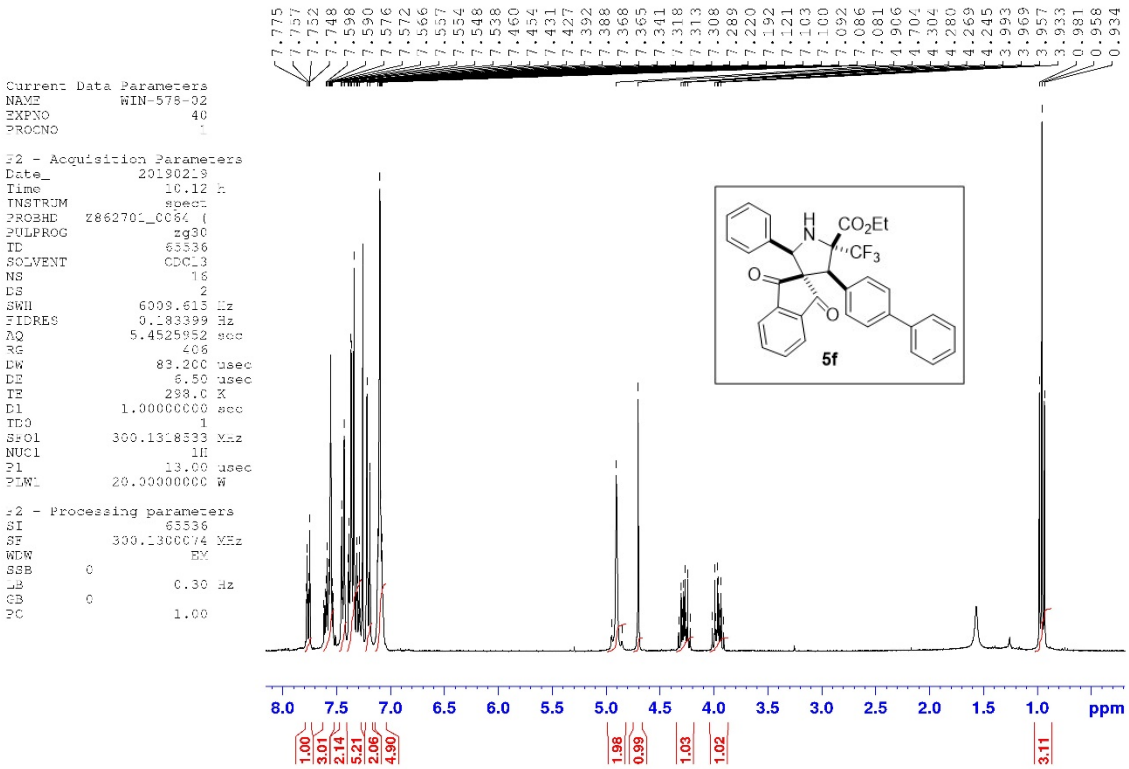

-74.503
Current Data Parameters
NAME WIN-583-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181126
Time 17.21 h
INSTRUM spect
PROBHD Z862701_CC84 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 2
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 645
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
H
N
CO2Et
CF3
O
O
NO2
5d
-70
-71
-72
-73
-74
-75
-76
-77
-78
-79
-80
ppm
3.00

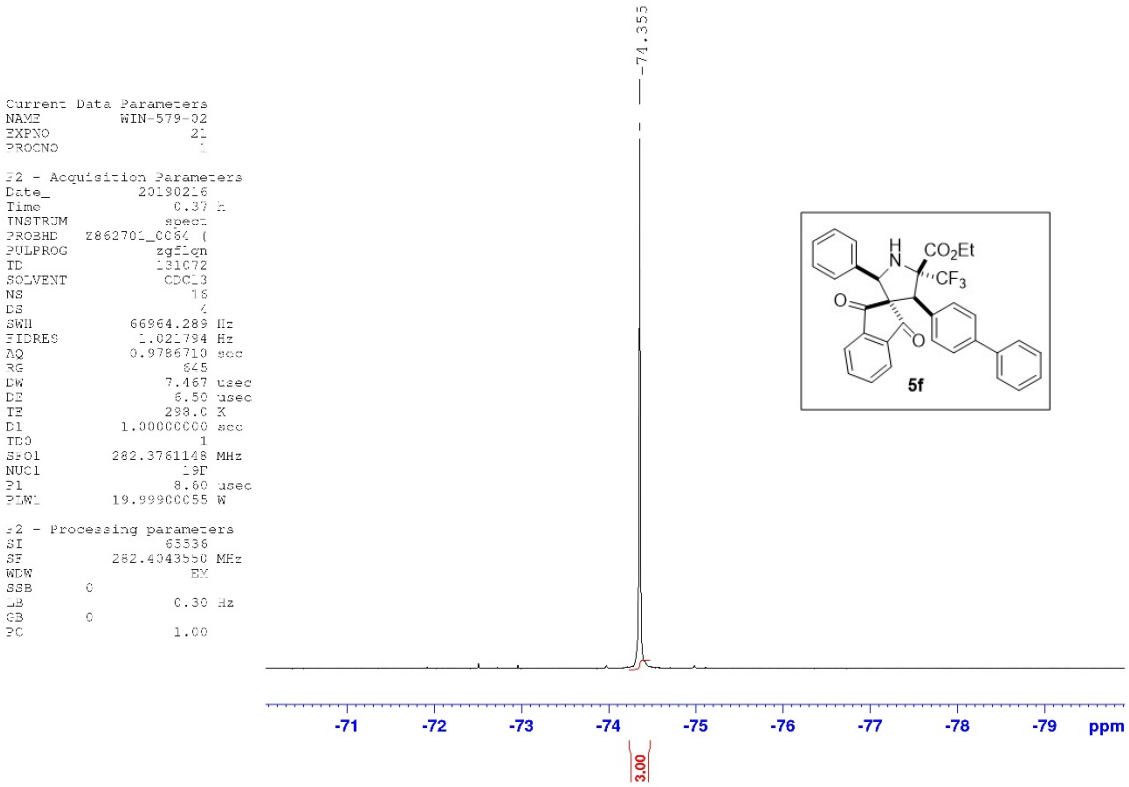

Current Data Parameters
NAME WIN-583-02
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190221
Time 1.55 h
INSTRUM spect
PROBHD Z862701_C084 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677386 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
199.088
198.368
166.226
147.745
142.254
141.938
141.088
136.279
136.044
132.778
131.546
128.802
128.552
127.639
126.582
123.376
123.124
123.051
74.688
74.368
72.355
72.138
58.965
13.594
CO2Et
CF3
NO2
5d
200
180
160
140
120
100
80
60
40
20
0
ppm

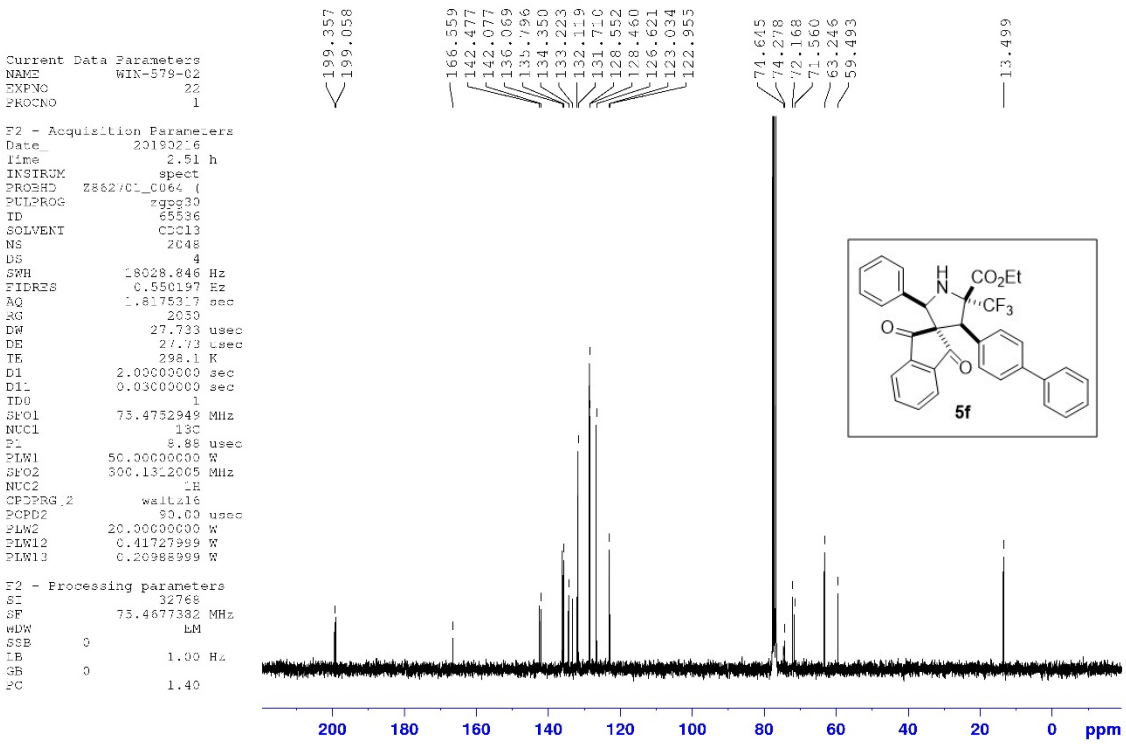

Current Data Parameters
NAME WIN-579-02
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190219
Time 10.18 h
INSTRUM spect
PROBHD Z862701_C084 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 456
DW 83.200 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.772
7.769
7.767
7.748
7.743
7.740
7.639
7.631
7.618
7.610
7.606
7.594
7.588
7.585
7.568
7.563
7.559
7.548
7.545
7.541
7.538
7.523
7.220
7.112
7.092
7.089
7.080
7.062
7.057
4.897
4.854
4.833
4.618
4.338
4.326
4.314
4.302
4.279
3.993
3.969
3.958
3.945
3.934
1.052
1.028
1.004
CO2Et
CF3
Cl
5e
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
3.07
9.16
2.06
1.03
1.06
1.03
3.16

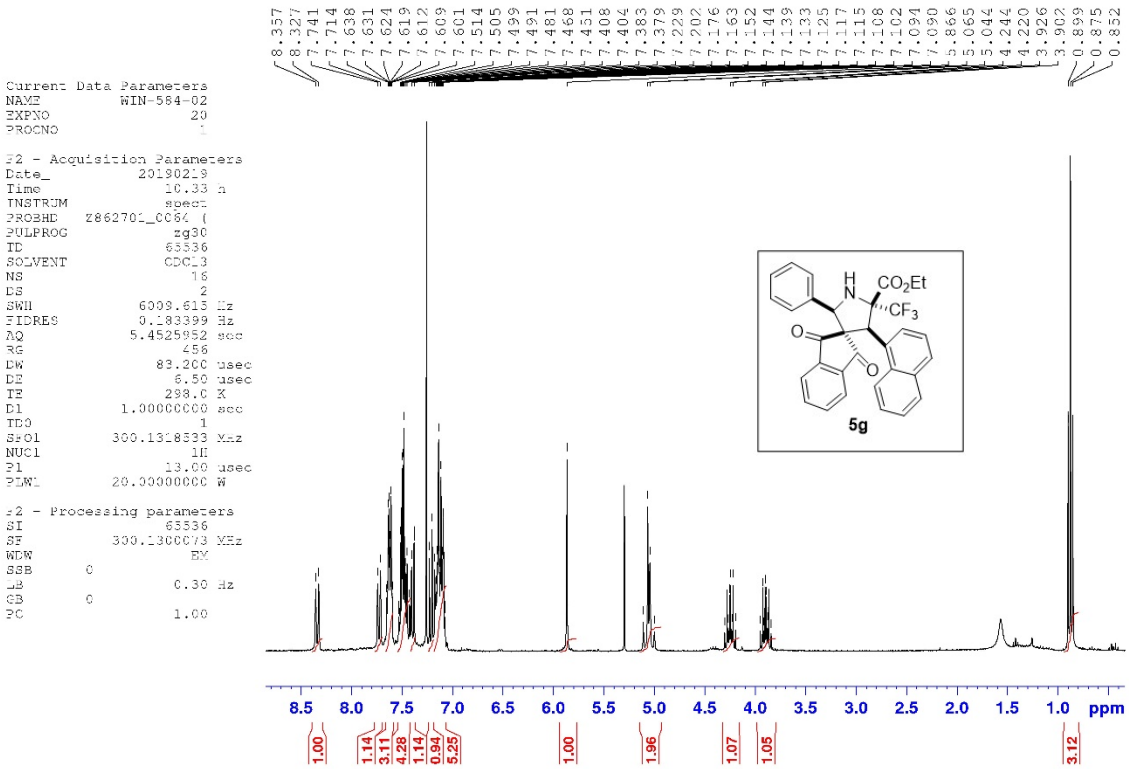

Current Data Parameters
NAME WIN-579-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181012
Time 13.29 h
INSTRUM spect
PROBHD Z862701_C084 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 645
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-74.354
CO2Et
CF3
Cl
5e
-71 -72 -73 -74 -75 -76 -77 -78 -79 ppm
3.00

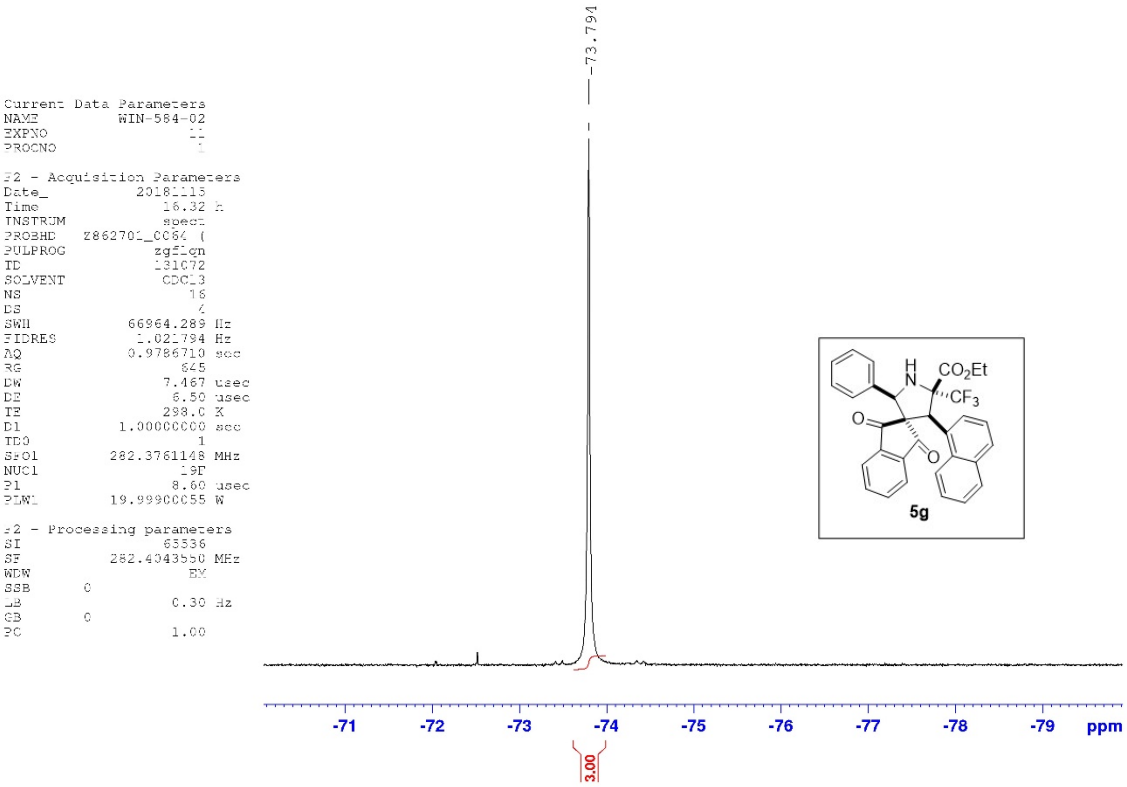

Current Data Parameters
NAME WIN-636-02
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190220
Time 21.21 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677389 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
199.426
199.316
166.625
142.583
141.955
136.187
135.841
134.254
133.248
132.244
130.126
128.645
128.422
128.337
128.071
127.804
124.025
123.048
75.072
74.704
74.340
73.975
71.733
70.267
63.140
60.969
13.339
CO2Et
CF3
Cl
5e
200 180 160 140 120 100 80 60 40 20 0 ppm

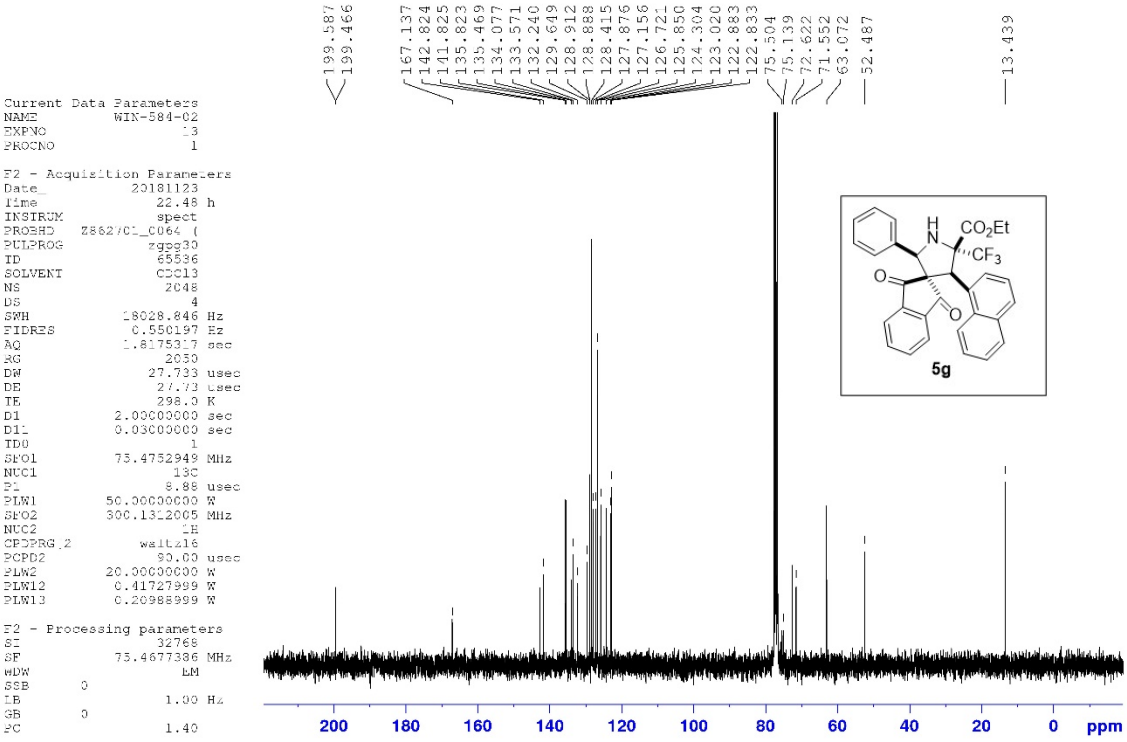

Current Data Parameters
NAME WIN-578-02
EXPNO 40
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190219
Time 10.12 h
INSTRUM spect
PROBHD Z862701_CC84 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 406
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.775
7.757
7.752
7.748
7.598
7.590
7.576
7.572
7.566
7.557
7.554
7.548
7.538
7.460
7.454
7.431
7.427
7.392
7.388
7.368
7.365
7.341
7.318
7.313
7.308
7.289
7.220
7.192
7.121
7.103
7.100
7.092
7.086
7.081
4.906
4.704
4.304
4.280
4.269
4.245
3.993
3.969
3.957
3.933
0.981
0.958
0.934
CO2Et
CF3
5f
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
3.01
2.14
5.21
2.06
4.90
1.98
0.99
1.03
1.02
3.11

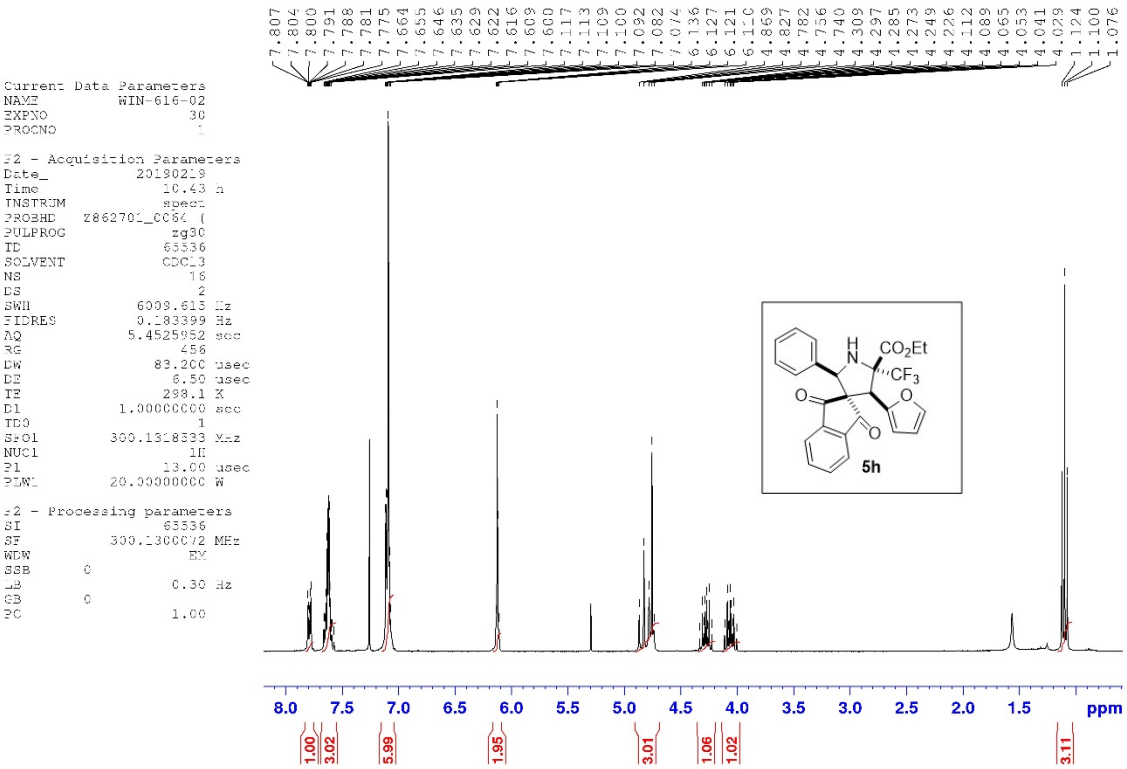

Current Data Parameters
NAME WIN-579-02
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190216
Time 0.37 h
INSTRUM spect
PROBHD Z862701_CC84 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 2
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 645
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-74.355
CO2Et
CF3
5f
-71
-72
-73
-74
-75
-76
-77
-78
-79
ppm
3.00

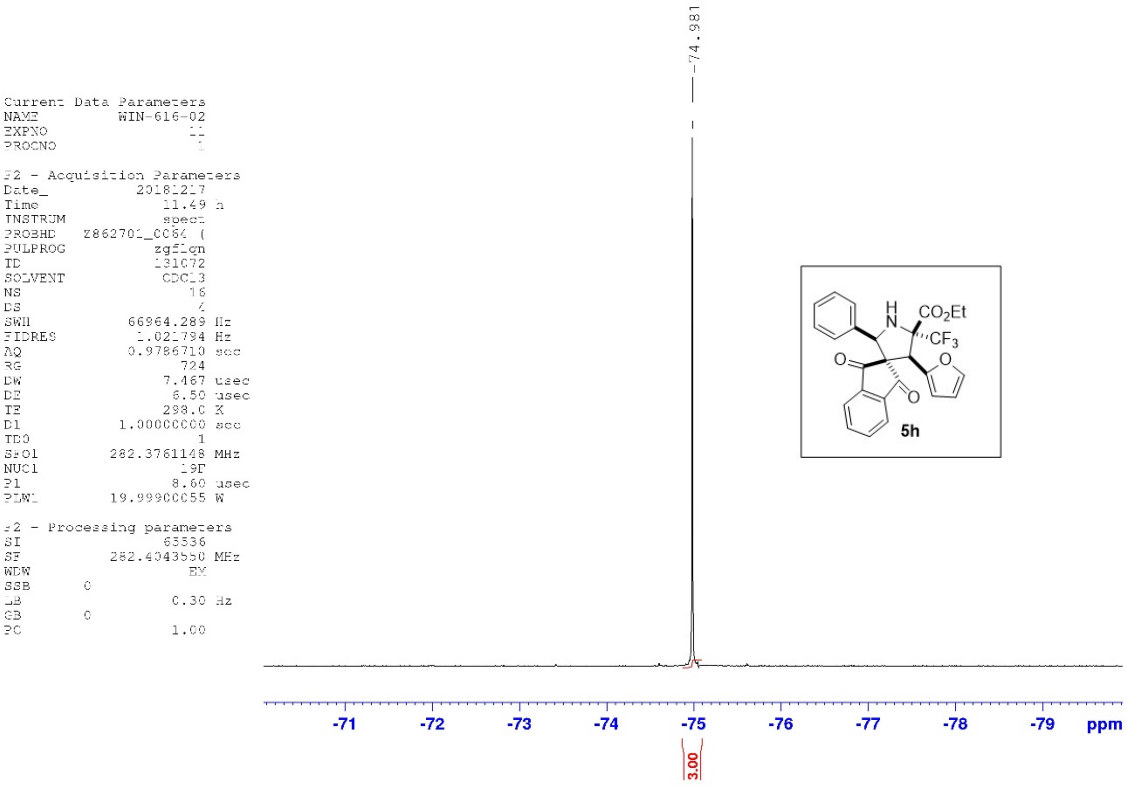

Current Data Parameters
NAME WIN-579-02
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190216
Time 2.51 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677382 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
199.357
199.058
166.559
142.477
142.077
136.069
135.796
134.350
133.223
132.119
131.710
128.552
128.460
126.621
123.034
122.955
74.645
74.278
72.168
71.560
63.246
59.493
13.499
5f
200
180
160
140
120
100
80
60
40
20
0
ppm

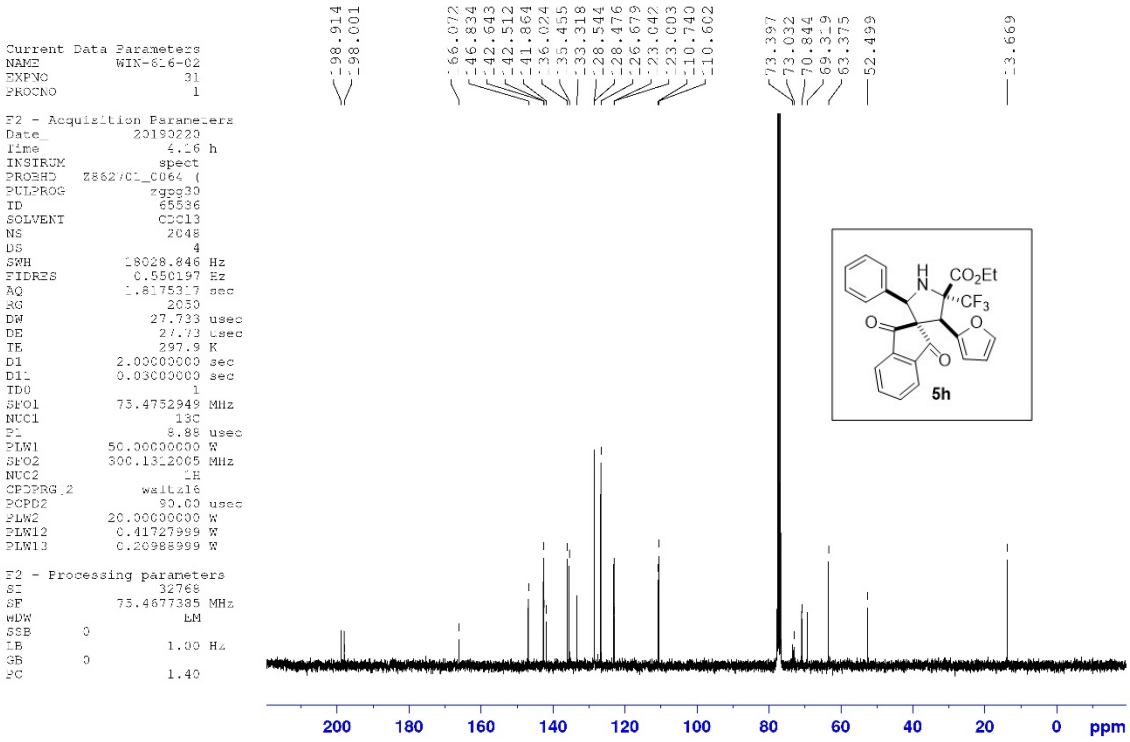

Current Data Parameters
NAME WIN-584-02
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190219
Time 10.33 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 456
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.357
8.327
7.741
7.714
7.638
7.631
7.624
7.619
7.612
7.609
7.601
7.514
7.505
7.499
7.491
7.481
7.468
7.451
7.408
7.404
7.383
7.379
7.229
7.202
7.176
7.163
7.152
7.144
7.139
7.133
7.125
7.117
7.115
7.108
7.102
7.094
7.090
5.866
5.065
5.044
4.244
4.220
3.926
3.902
0.899
0.875
0.852
5g
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.14
3.11
4.28
1.14
0.94
5.25
1.00
1.96
1.07
1.05
3.12

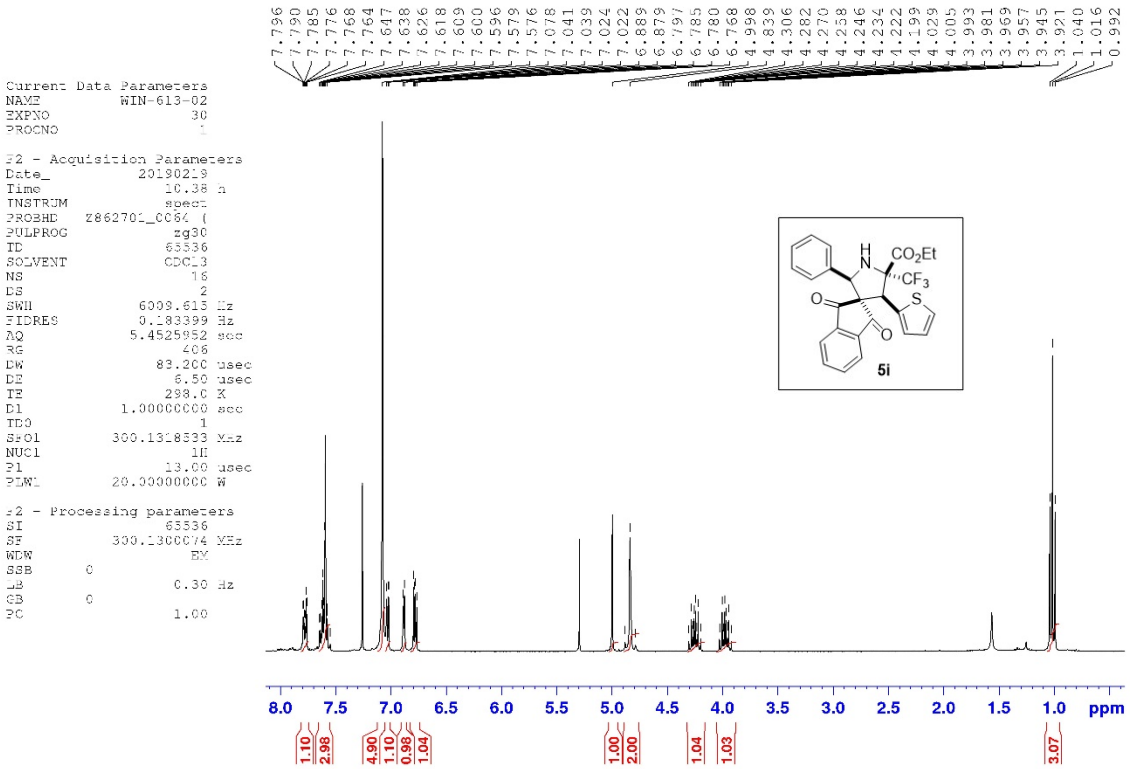

Current Data Parameters
NAME WIN-584-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181115
Time 16.32 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 645
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-73.794
5g
-71
-72
-73
-74
-75
-76
-77
-78
-79
ppm
3.00

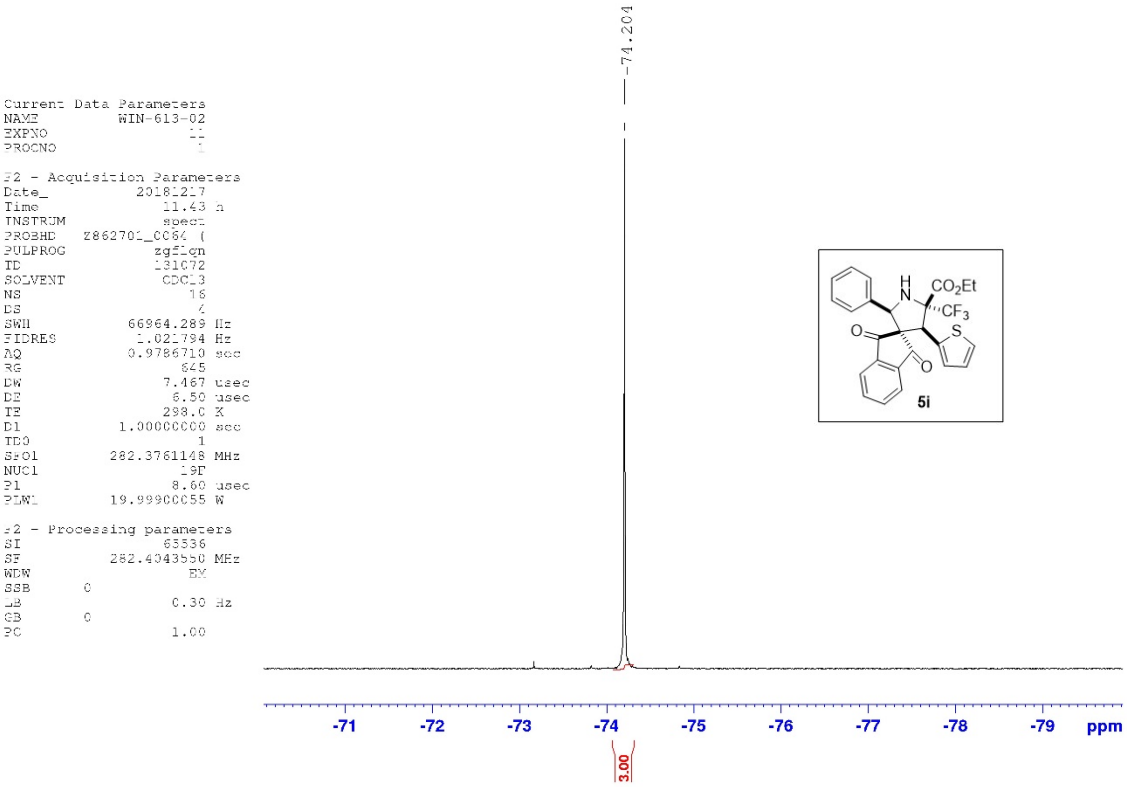

199.587
199.466
167.137
142.824
141.825
135.823
135.469
134.077
133.571
132.240
129.649
128.912
128.888
128.415
127.876
127.156
126.721
125.850
124.304
123.020
122.883
122.833
75.504
75.139
72.622
71.552
63.072
52.487
13.439
Current Data Parameters
NAME WIN-584-02
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181123
Time 22.48 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677386 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
5g
200
180
160
140
120
100
80
60
40
20
0
ppm

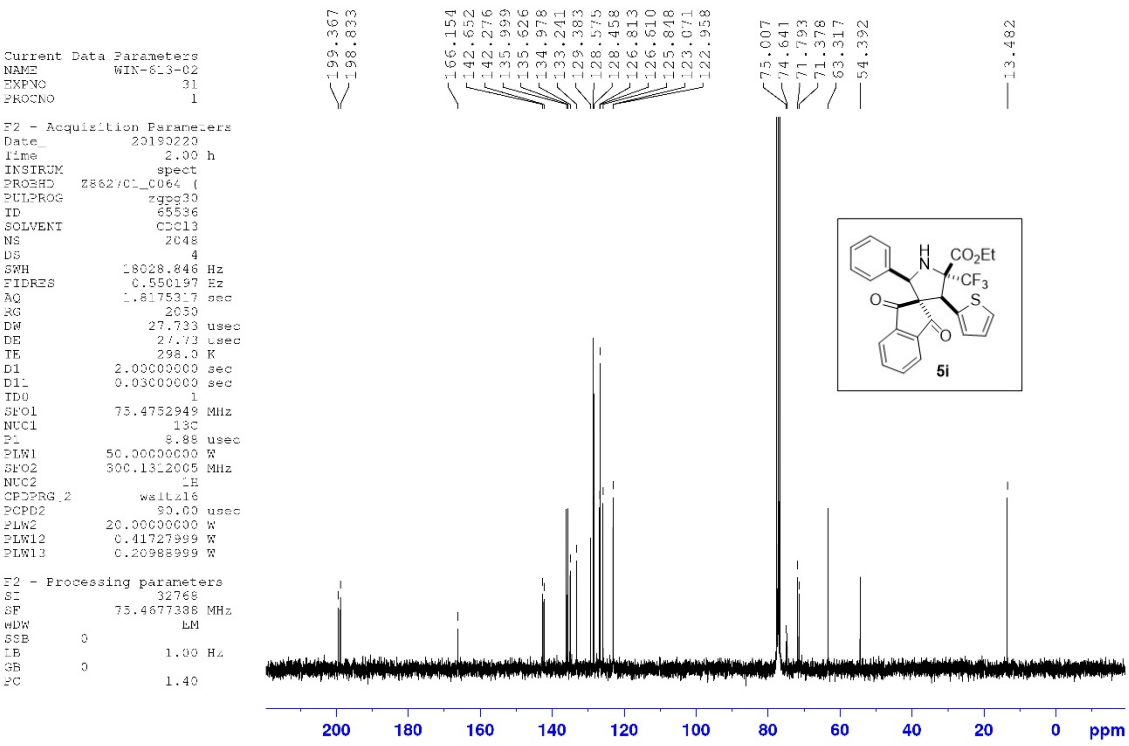

Current Data Parameters
NAME WIN-616-02
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190219
Time 10.43 h
INSTRUM spect
PROBHD Z862701_CC84 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 456
DW 83.200 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.807 7.804 7.800 7.791 7.788 7.781 7.775 7.664 7.655 7.646 7.635 7.629 7.622 7.616 7.609 7.600 7.117 7.113 7.109 7.100 7.092 7.082 7.074 6.136 6.127 6.121 6.110 4.869 4.827 4.782 4.756 4.740 4.309 4.297 4.285 4.273 4.249 4.226 4.112 4.089 4.065 4.053 4.041 4.029 1.124 1.100 1.076
CO2Et
CF3
5h
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
1.00 3.02 5.99 1.95 3.01 1.06 1.02 3.11

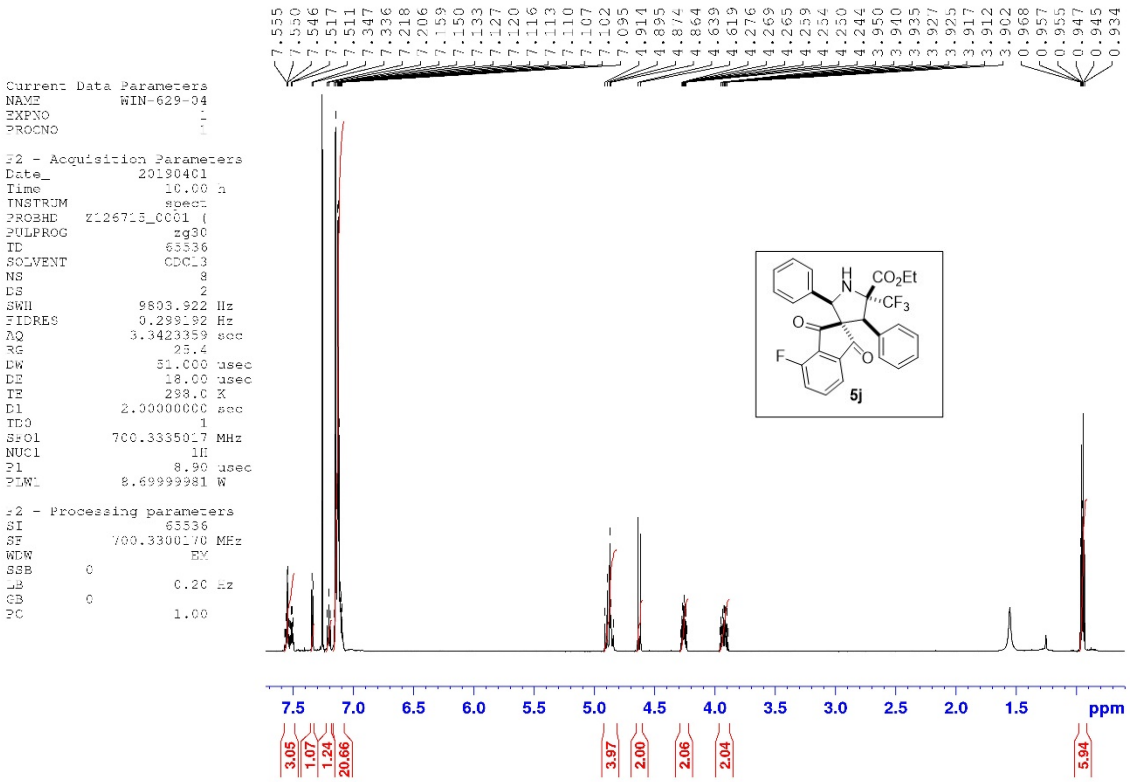

Current Data Parameters
NAME WIN-616-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181217
Time 11.49 h
INSTRUM spect
PROBHD Z862701_CC84 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 2
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 724
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-74.981
CO2Et
CF3
5h
-71 -72 -73 -74 -75 -76 -77 -78 -79 ppm
3.00

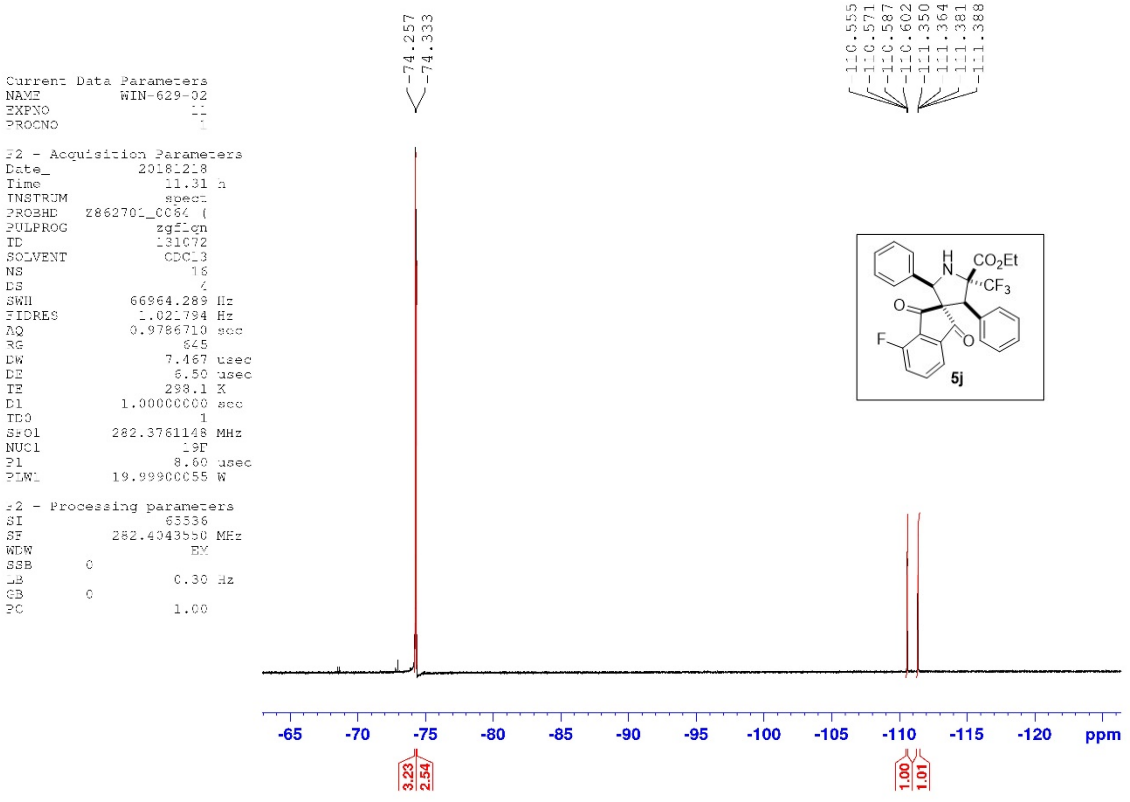

Current Data Parameters
NAME WIN-816-02
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190220
Time 4.16 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2030
DW 27.733 usec
DE 27.73 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677385 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
98.914
98.001
66.072
46.834
42.643
42.512
41.864
36.024
35.455
33.318
28.544
28.476
26.679
23.042
23.003
10.740
10.602
73.397
73.032
70.844
69.329
63.375
52.499
13.669
CO2Et
CF3
5h
200
180
160
140
120
100
80
60
40
20
0
ppm

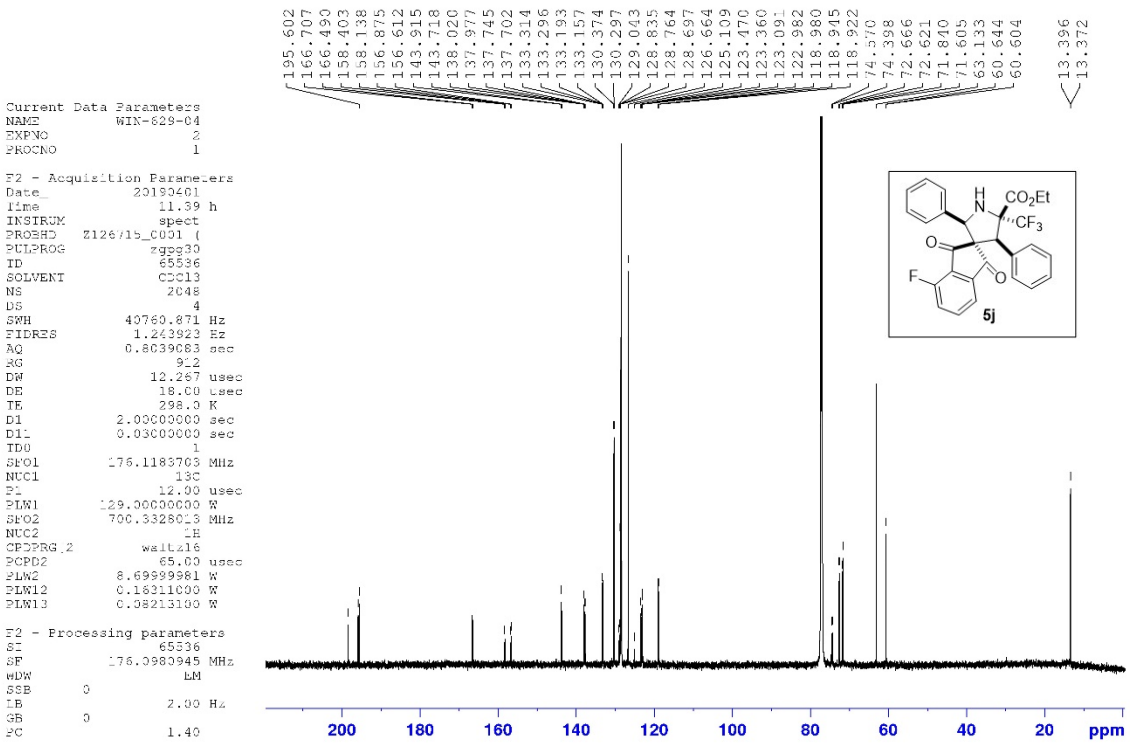

Current Data Parameters
NAME WIN-613-02
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190219
Time 10.38 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 406
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.796
7.790
7.785
7.776
7.768
7.764
7.647
7.638
7.626
7.618
7.609
7.600
7.596
7.579
7.576
7.078
7.041
7.039
7.024
7.022
6.889
6.879
6.797
6.785
6.780
6.768
4.998
4.839
4.306
4.282
4.270
4.258
4.246
4.234
4.222
4.199
4.029
4.005
3.993
3.981
3.969
3.957
3.945
3.921
1.040
1.016
0.992
CO2Et
CF3
5i
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.10
2.98
4.90
1.10
0.98
1.04
1.00
2.00
1.04
1.03
3.07

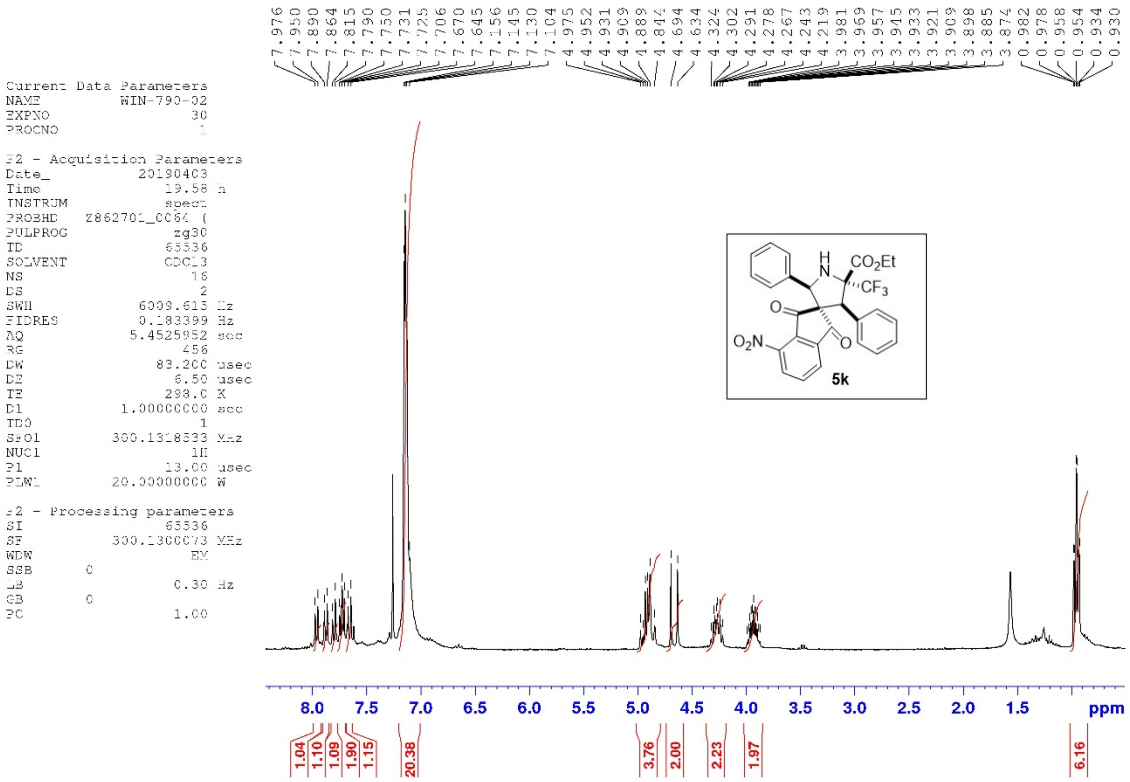

Current Data Parameters
NAME WIN-613-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181217
Time 11.43 h
INSTRUM spect
PROBHD Z862701_C084 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 645
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-74.204
CO2Et
CF3
5i
-71
-72
-73
-74
-75
-76
-77
-78
-79
ppm
3.00

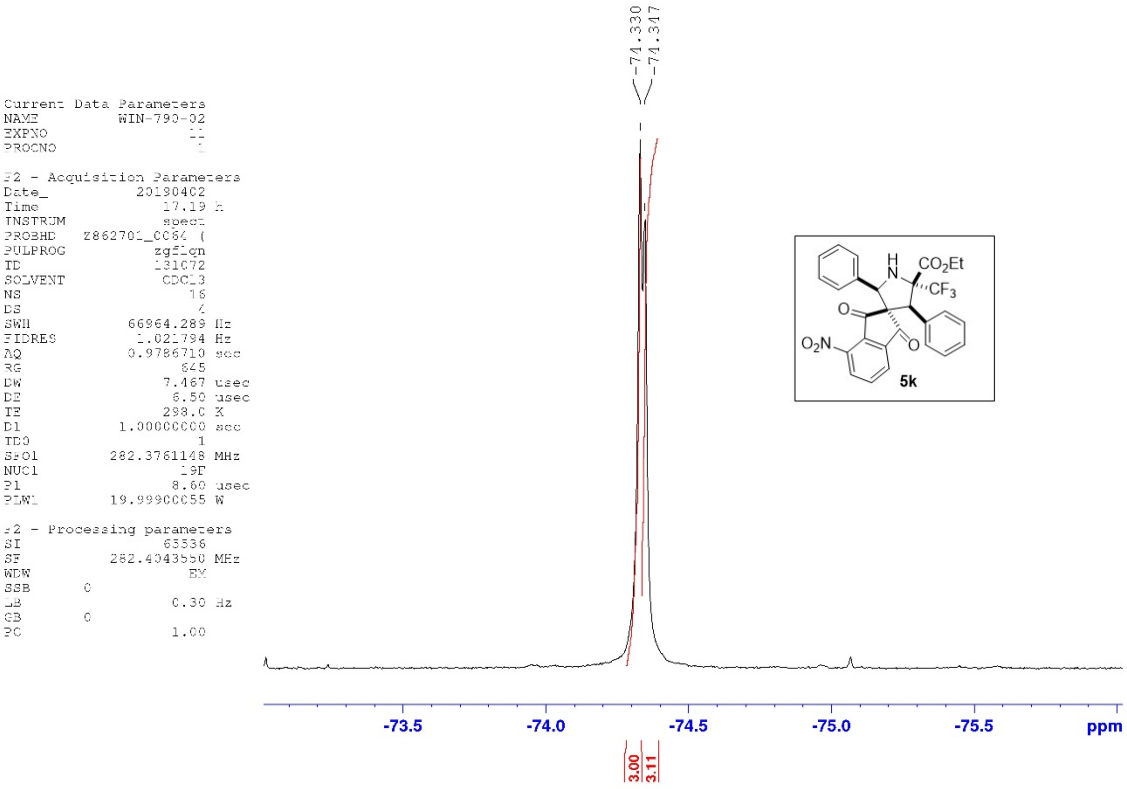

Current Data Parameters
NAME WIN-613-02
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190220
Time 2.00 h
INSTRUM spect
PROBHD Z862701_C084 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677388 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
199.367
198.833
166.154
142.652
142.276
135.999
135.626
134.978
133.241
129.383
128.575
128.458
126.813
126.610
125.848
123.071
122.958
75.007
74.641
71.793
71.378
63.317
54.392
13.482
CO2Et
CF3
5i
200
180
160
140
120
100
80
60
40
20
0
ppm

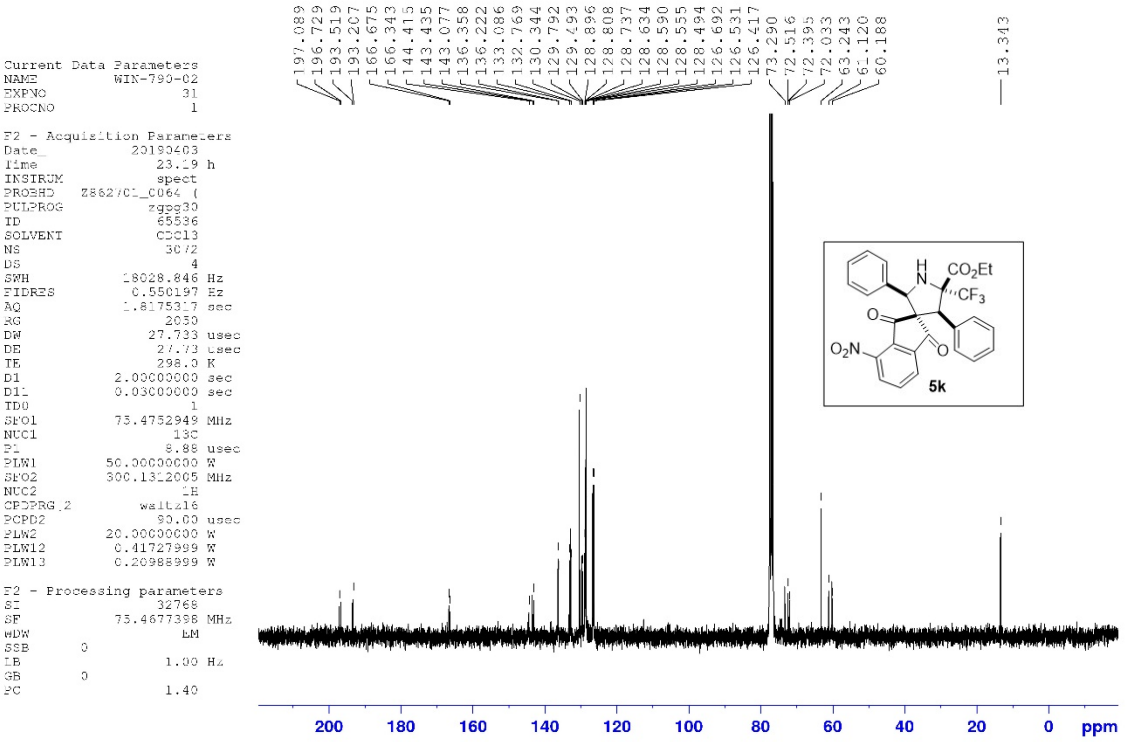

Current Data Parameters
NAME WIN-629-04
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190401
Time 10.00 h
INSTRUM spect
PROBHD Z126715_C001 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 9803.922 Hz
FIDRES 0.299192 Hz
AQ 3.3423359 sec
RG 25.4
DW 51.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
SFO1 700.3335017 MHz
NUC1 1H
P1 8.90 usec
PLW1 8.69999981 W
F2 - Processing parameters
SI 65536
SF 700.3300170 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
7.555
7.550
7.546
7.517
7.511
7.347
7.336
7.218
7.206
7.159
7.150
7.133
7.127
7.120
7.116
7.113
7.110
7.107
7.102
7.095
4.914
4.895
4.874
4.864
4.639
4.619
4.276
4.269
4.265
4.259
4.254
4.250
4.244
3.950
3.940
3.935
3.927
3.925
3.917
3.912
3.902
0.968
0.957
0.955
0.947
0.945
0.934
CO2Et
CF3
O
F
O
5j
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
3.05
1.07
1.24
20.66
3.97
2.00
2.06
2.04
5.94

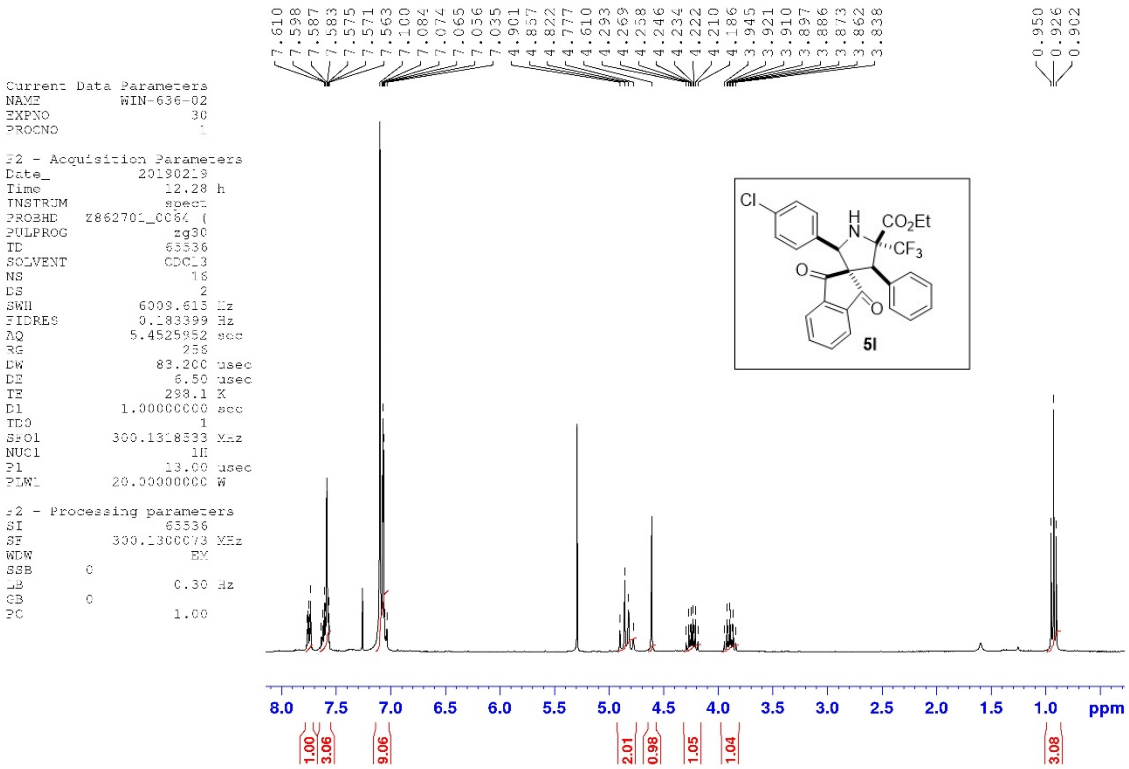

Current Data Parameters
NAME WIN-629-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181218
Time 11.31 h
INSTRUM spect
PROBHD Z862701_C084 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 645
DW 7.467 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-74.257
-74.333
-110.555
-110.571
-110.587
-110.602
-111.350
-111.364
-111.381
-111.388
CO2Et
CF3
O
F
O
5j
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
ppm
3.23
2.54
1.00
1.01

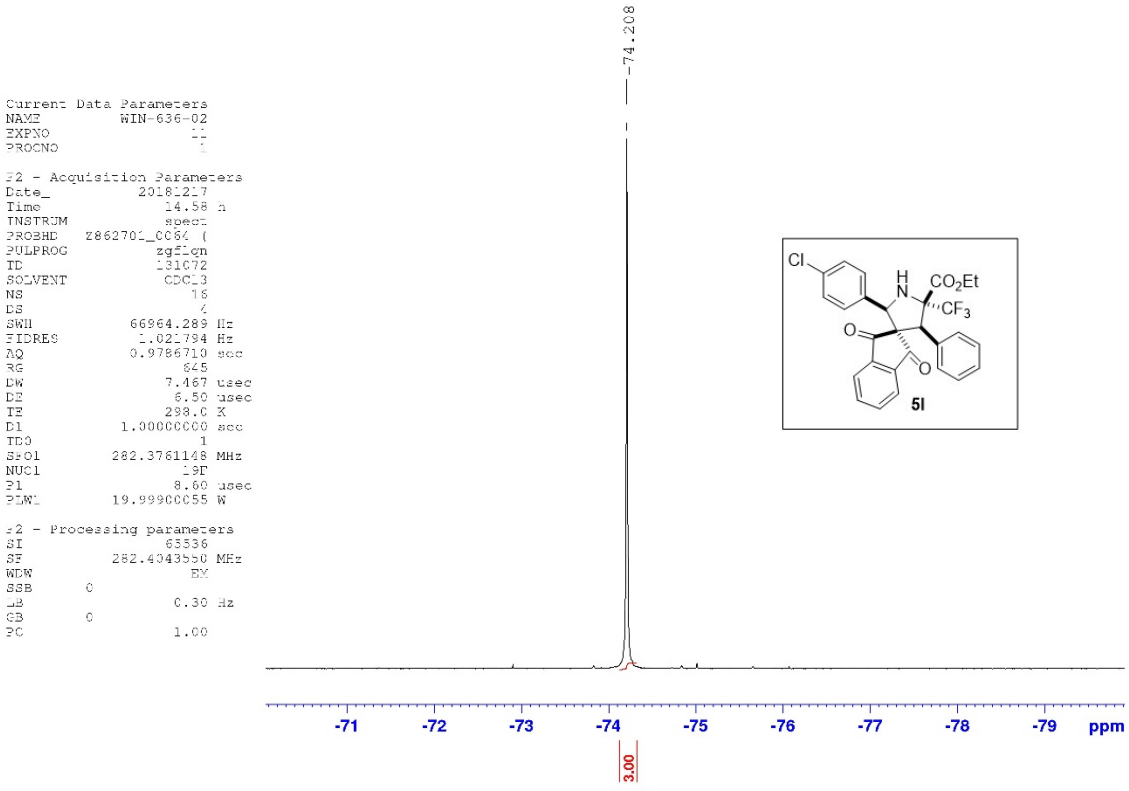

195.602
166.707
166.490
158.403
158.138
156.875
156.612
143.915
143.718
138.020
137.977
137.745
137.702
133.314
133.296
133.193
133.157
130.374
130.297
129.043
128.835
128.764
128.697
126.664
125.109
123.470
123.360
123.091
122.982
118.980
118.945
118.922
74.570
74.398
72.666
72.621
71.840
71.605
63.133
60.644
60.604
13.396
13.372
Current Data Parameters
NAME WIN-629-04
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190401
Time 11.39 h
INSTRUM spect
PROBHD Z126715_C001 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 40760.871 Hz
FIDRES 1.243923 Hz
AQ 0.8039083 sec
RG 912
DW 12.267 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 176.1183703 MHz
NUC1 13C
P1 12.00 usec
PLW1 129.00000000 W
SFO2 700.3328013 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 65.00 usec
PLW2 8.69999981 W
PLW12 0.18311000 W
PLW13 0.08213100 W
F2 - Processing parameters
SI 65536
SF 176.0980945 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
CO2Et
CF3
O
F
O
5j
200
180
160
140
120
100
80
60
40
20
ppm

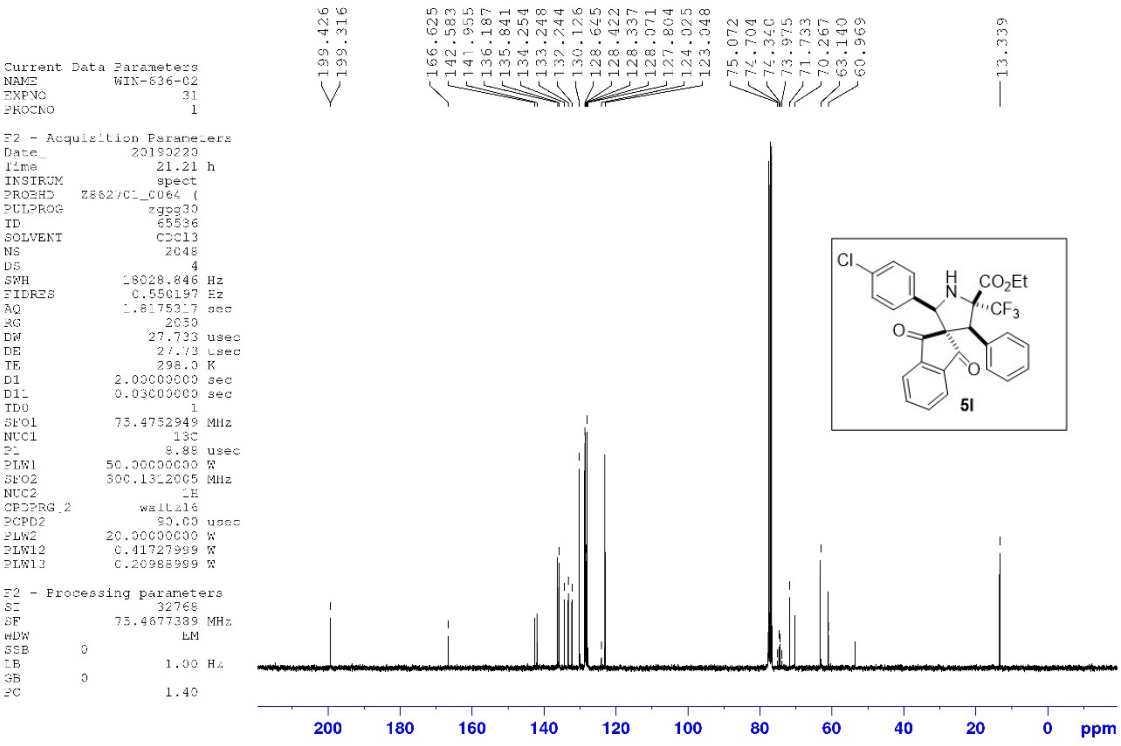

7.976
7.950
7.890
7.864
7.815
7.790
7.750
7.731
7.725
7.706
7.670
7.645
7.156
7.145
7.130
7.104
4.975
4.952
4.931
4.909
4.889
4.842
4.694
4.634
4.324
4.302
4.291
4.278
4.267
4.243
4.219
3.981
3.969
3.957
3.945
3.933
3.921
3.909
3.898
3.885
3.874
0.982
0.978
0.958
0.954
0.934
0.930
Current Data Parameters
NAME WIN-790-02
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190403
Time 19.58 h
INSTRUM spect
PROBHD Z862701_C084 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 456
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CO2Et
CF3
O
O2N
O
5k
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.04
1.10
1.09
1.90
1.15
20.38
3.76
2.00
2.23
1.97
6.16

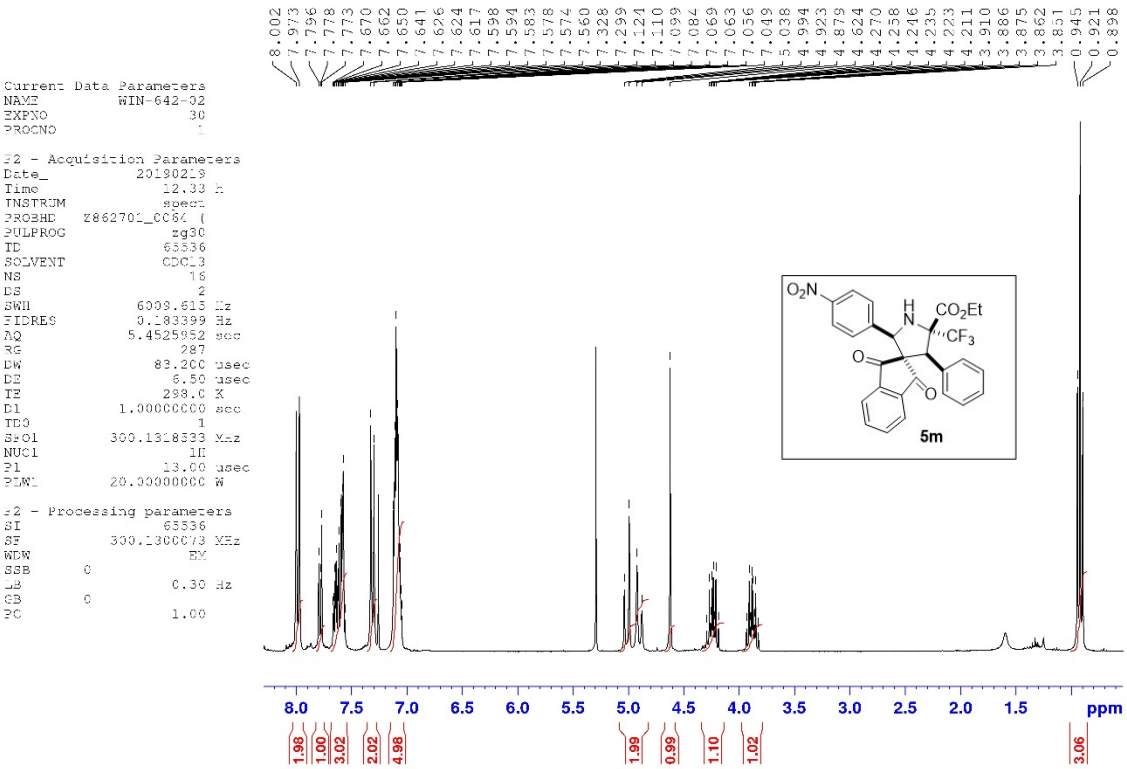

Current Data Parameters
NAME WIN-790-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190402
Time 17.19 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 645
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-74.330
-74.347
5k
-73.5
-74.0
-74.5
-75.0
-75.5
ppm
3.00
3.11

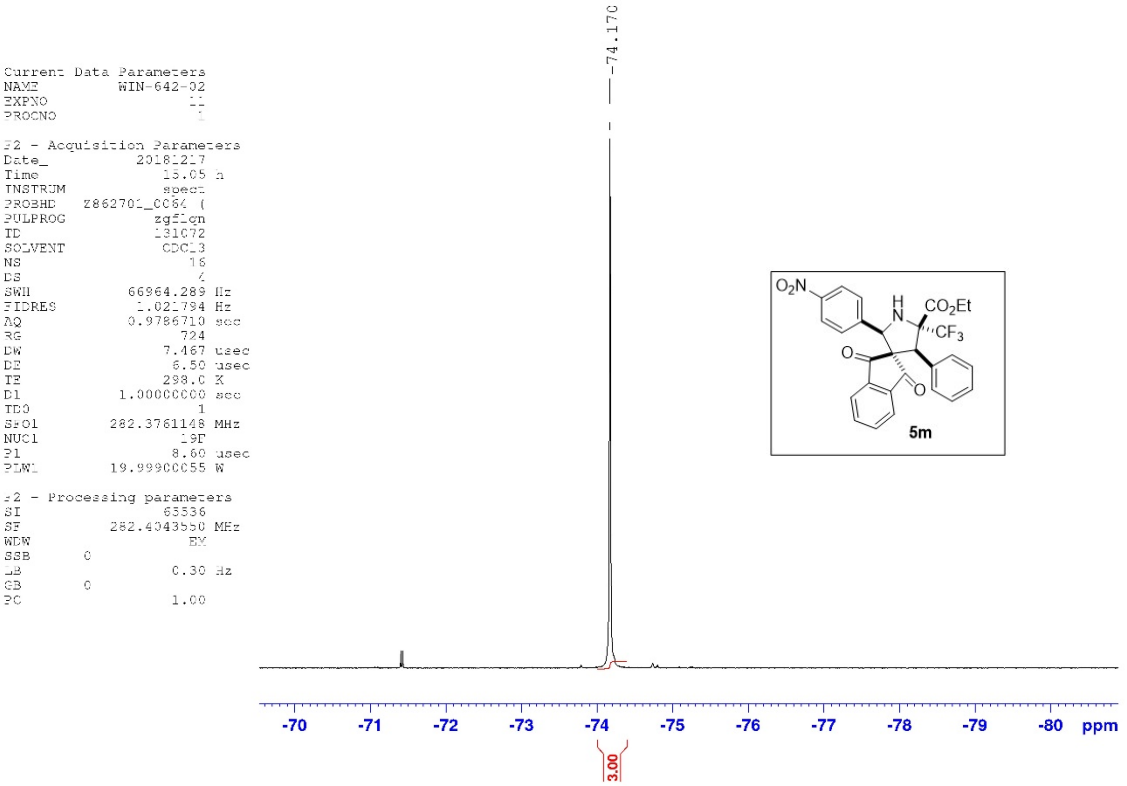

Current Data Parameters
NAME WIN-790-02
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190403
Time 23.29 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677398 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
197.089
196.729
193.519
193.207
166.675
166.343
144.415
143.435
143.077
136.358
136.222
133.086
132.769
130.344
129.792
129.293
128.896
128.808
128.737
128.634
128.590
128.555
128.494
126.692
126.531
126.417
73.290
72.516
72.395
72.033
63.243
61.120
60.188
13.343
5k
200
180
160
140
120
100
80
60
40
20
0
ppm

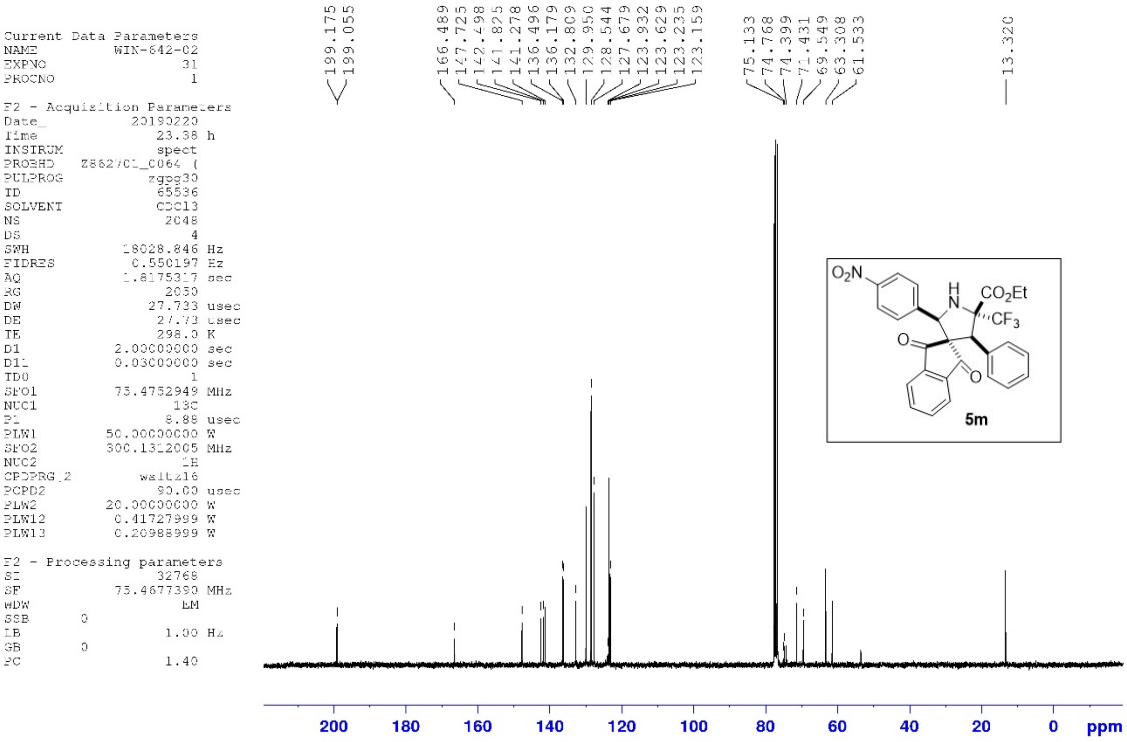

7.610
7.598
7.587
7.583
7.575
7.571
7.563
7.100
7.084
7.074
7.065
7.056
7.035
4.901
4.857
4.822
4.777
4.610
4.293
4.269
4.258
4.246
4.234
4.222
4.210
4.186
3.945
3.921
3.910
3.897
3.886
3.873
3.862
3.838
0.950
0.926
0.902
Current Data Parameters
NAME WIN-636-02
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190219
Time 12.28 h
INSTRUM spect
PROBHD Z862701_CC84 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 258
DW 83.200 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
H
N
CO2Et
CF3
O
O
5l
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
3.06
9.06
2.01
0.98
1.05
1.04
3.08

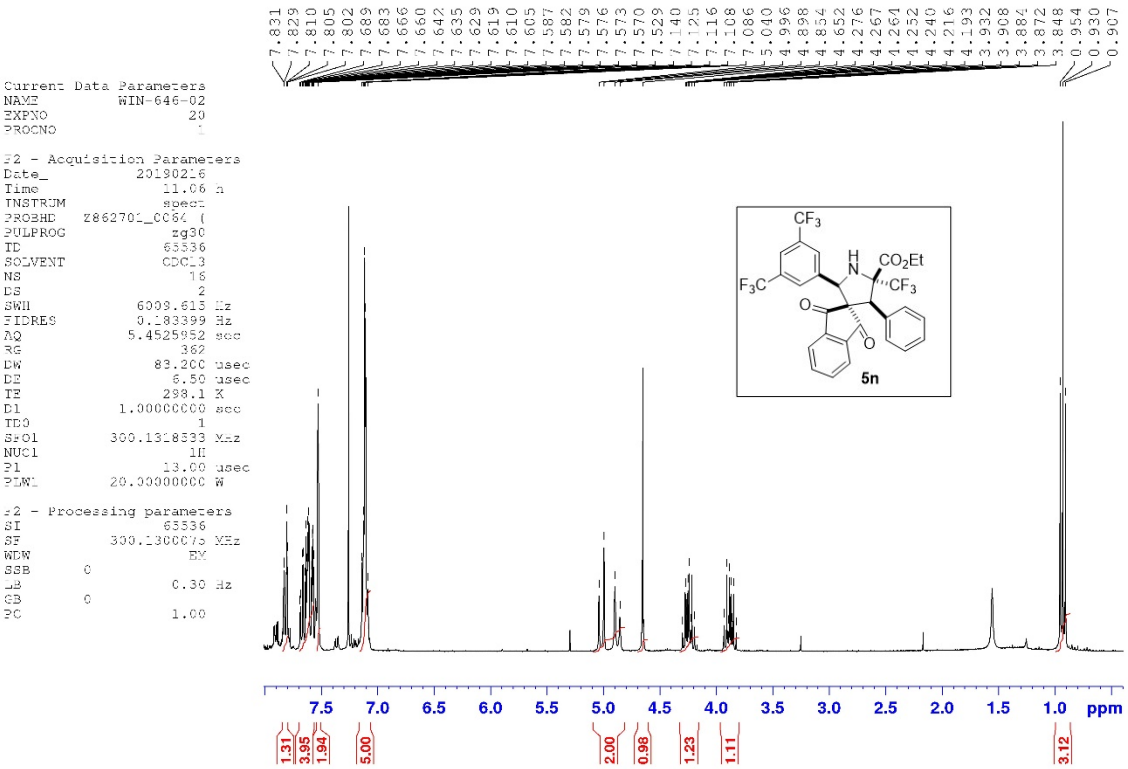

-74.208
Current Data Parameters
NAME WIN-636-02
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181217
Time 14.58 h
INSTRUM spect
PROBHD Z862701_CC84 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 2
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 645
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
H
N
CO2Et
CF3
O
O
5l
-71
-72
-73
-74
-75
-76
-77
-78
-79
ppm
3.00

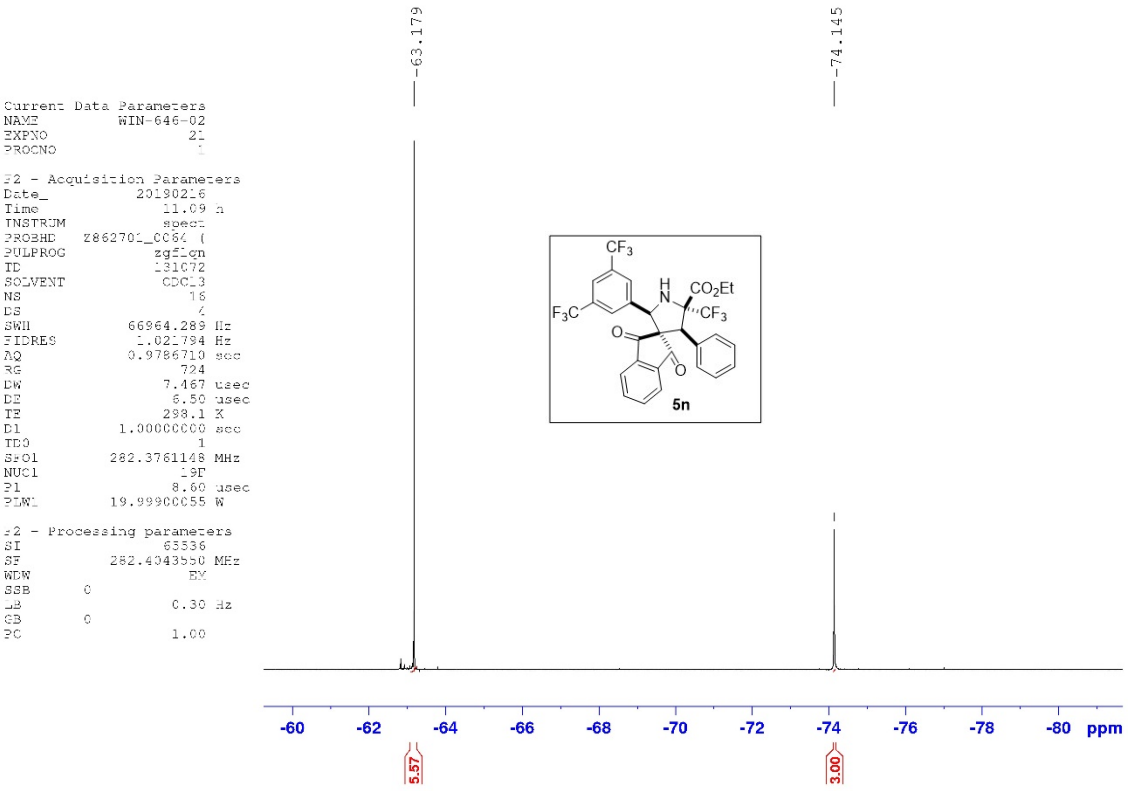

199.426
199.316
166.625
142.583
141.955
136.187
135.841
134.254
133.248
132.244
130.126
128.665
128.422
128.337
128.071
127.804
124.025
123.048
75.072
74.704
74.340
73.975
71.733
70.267
63.140
60.969
13.339
Current Data Parameters
NAME WIN-636-02
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190220
Time 21.21 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677389 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Cl
H
N
CO2Et
CF3
O
O
5l
200
180
160
140
120
100
80
60
40
20
0
ppm

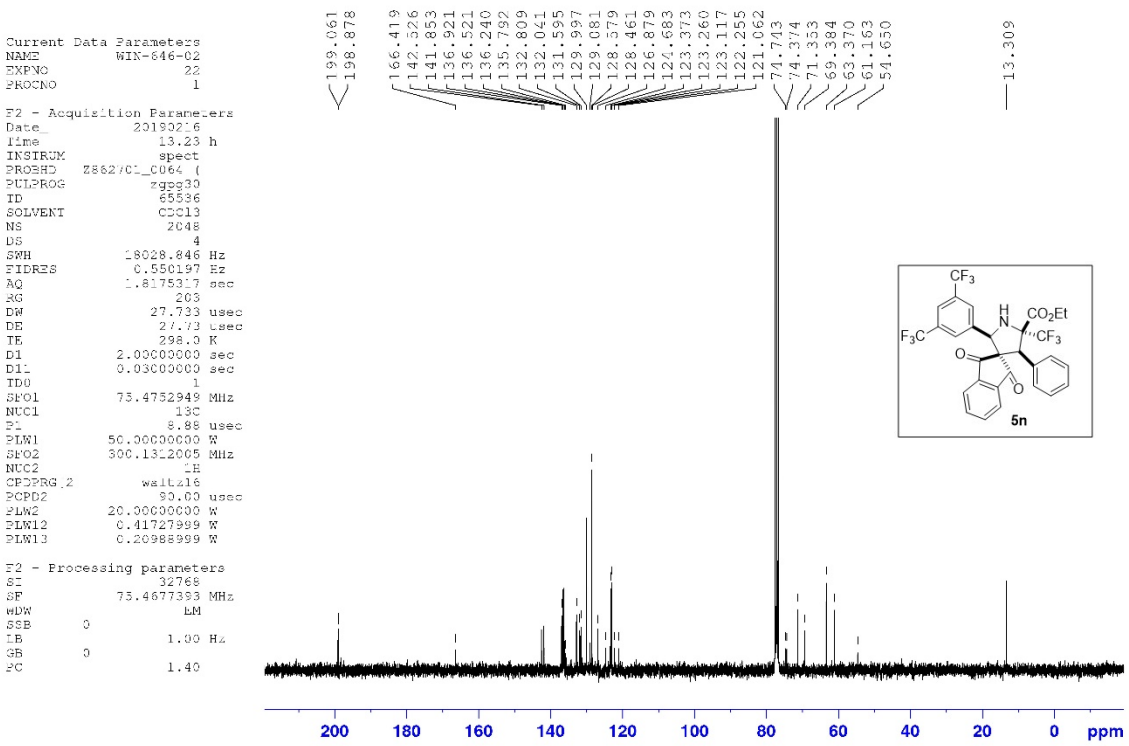

8.002
7.973
7.796
7.778
7.773
7.670
7.662
7.650
7.641
7.626
7.624
7.617
7.598
7.594
7.583
7.578
7.574
7.560
7.328
7.299
7.124
7.110
7.099
7.082
7.069
7.063
7.056
7.049
5.038
4.994
4.923
4.879
4.624
4.270
4.258
4.246
4.235
4.223
4.211
3.910
3.886
3.875
3.862
3.851
0.945
0.921
0.898
Current Data Parameters
NAME WIN-642-02
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190219
Time 12.33 h
INSTRUM spect
PROBHD Z862701_C064 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 287
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 300.1328533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O2N
H
N
CO2Et
CF3
O
O
5m
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.98
1.00
3.02
2.02
4.98
1.99
0.99
1.10
1.02
3.06

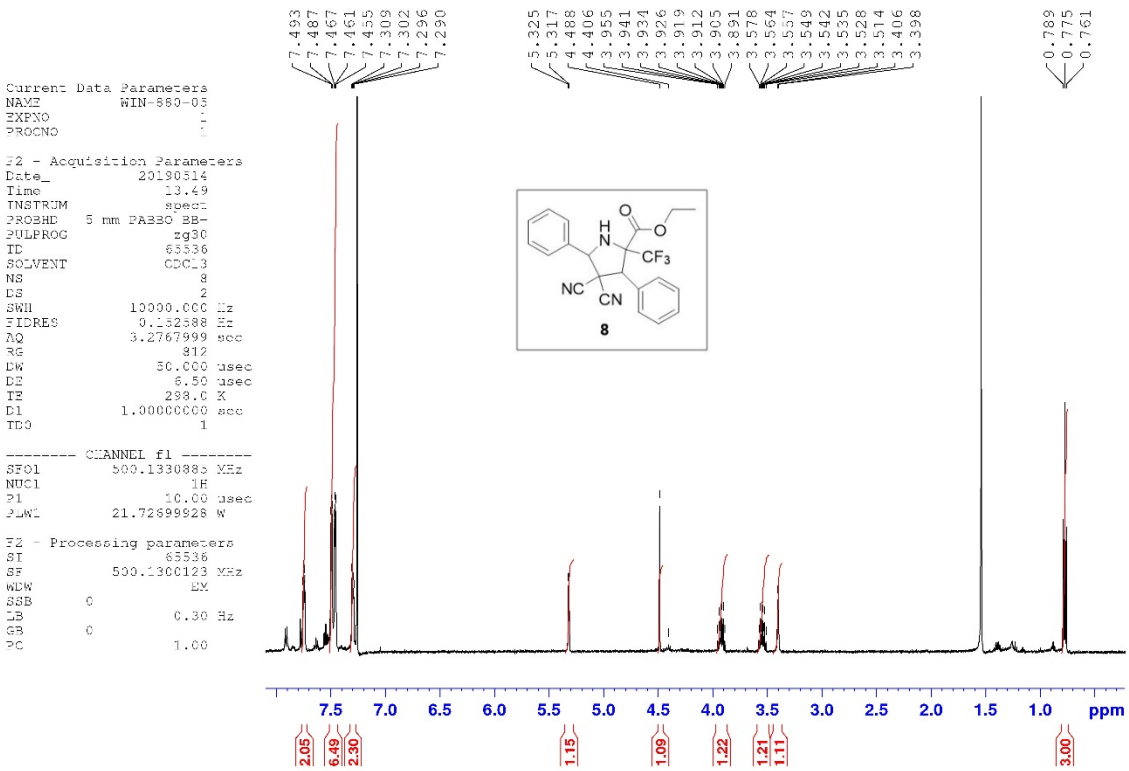

Current Data Parameters
NAME WIN-642-02
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181217
Time 13.05 h
INSTRUM spect
PROBHD Z862701_C084 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 724
DW 7.467 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-74.170
O2N
CO2Et
CF3
5m
-70 -71 -72 -73 -74 -75 -76 -77 -78 -79 -80 ppm
3.00

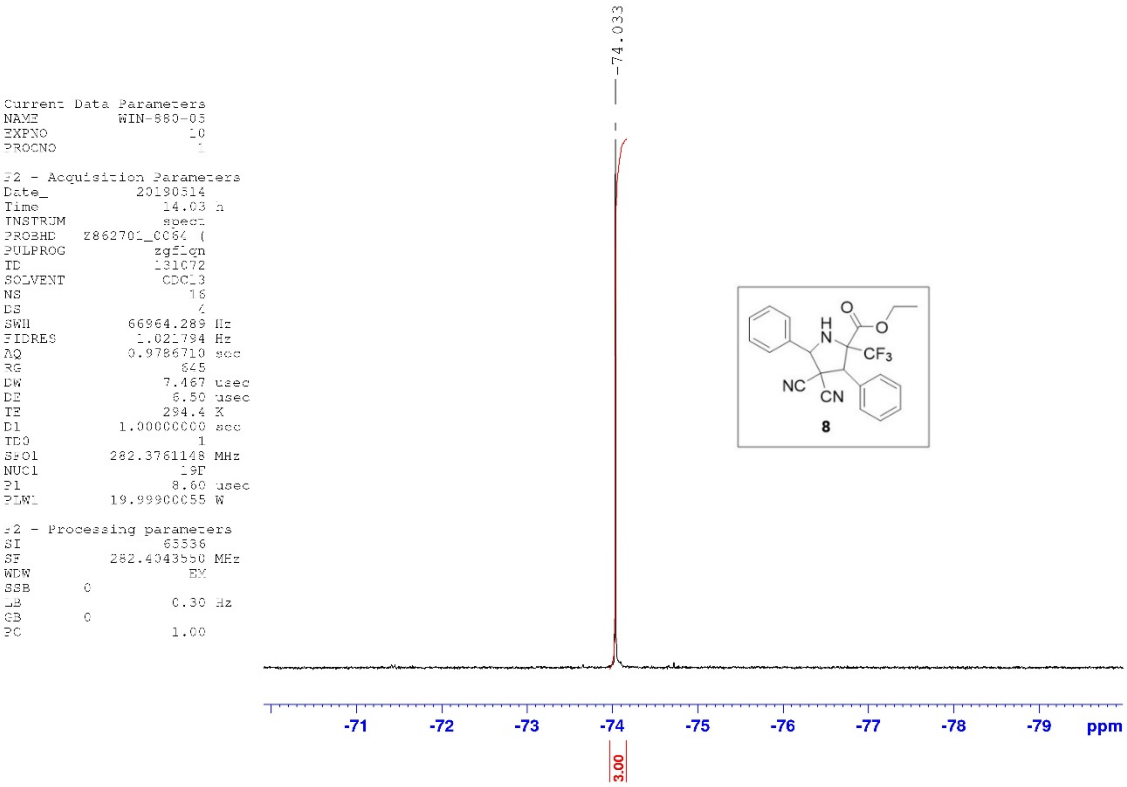

Current Data Parameters
NAME WIN-642-02
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190220
Time 23.38 h
INSTRUM spect
PROBHD Z862701_C084 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 2050
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
199.175
199.055
166.489
147.725
142.498
141.825
141.278
136.496
136.179
132.809
129.950
128.544
127.679
123.932
123.629
123.235
123.159
75.133
74.768
74.399
72.431
69.549
63.308
61.533
13.320
O2N
CO2Et
CF3
5m
200 180 160 140 120 100 80 60 40 20 0 ppm

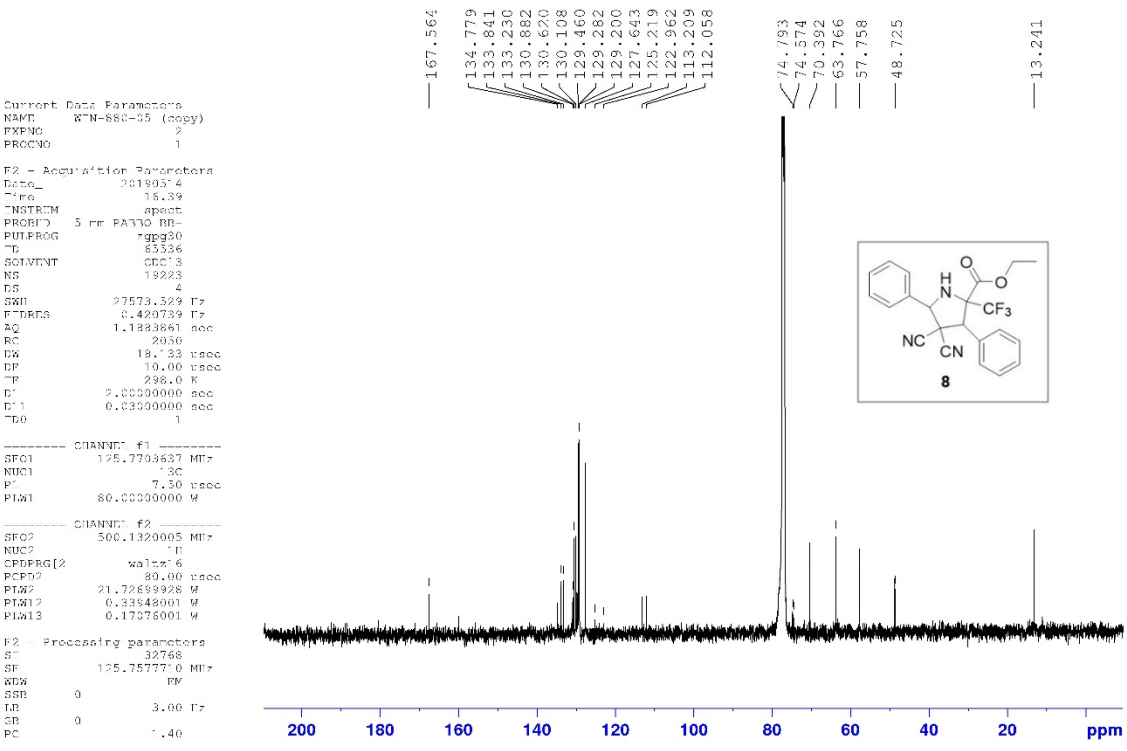

7.831
7.829
7.810
7.805
7.802
7.689
7.683
7.666
7.660
7.642
7.635
7.629
7.619
7.610
7.605
7.587
7.582
7.579
7.576
7.573
7.570
7.529
7.140
7.125
7.116
7.108
7.086
5.040
4.996
4.898
4.854
4.652
4.276
4.267
4.264
4.252
4.240
4.216
4.193
3.932
3.908
3.884
3.872
3.848
0.954
0.930
0.907
Current Data Parameters
NAME WIN-646-02
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190216
Time 11.06 h
INSTRUM spect
PROBHD Z862701_CC84 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 5.4525952 sec
RG 362
DW 83.200 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 300.1318533 MHz
NUC1 1H
P1 13.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 300.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CF3
F3C
H
N
CO2Et
CF3
O
O
5n
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.31
3.95
1.94
5.00
2.00
0.98
1.23
1.11
3.12

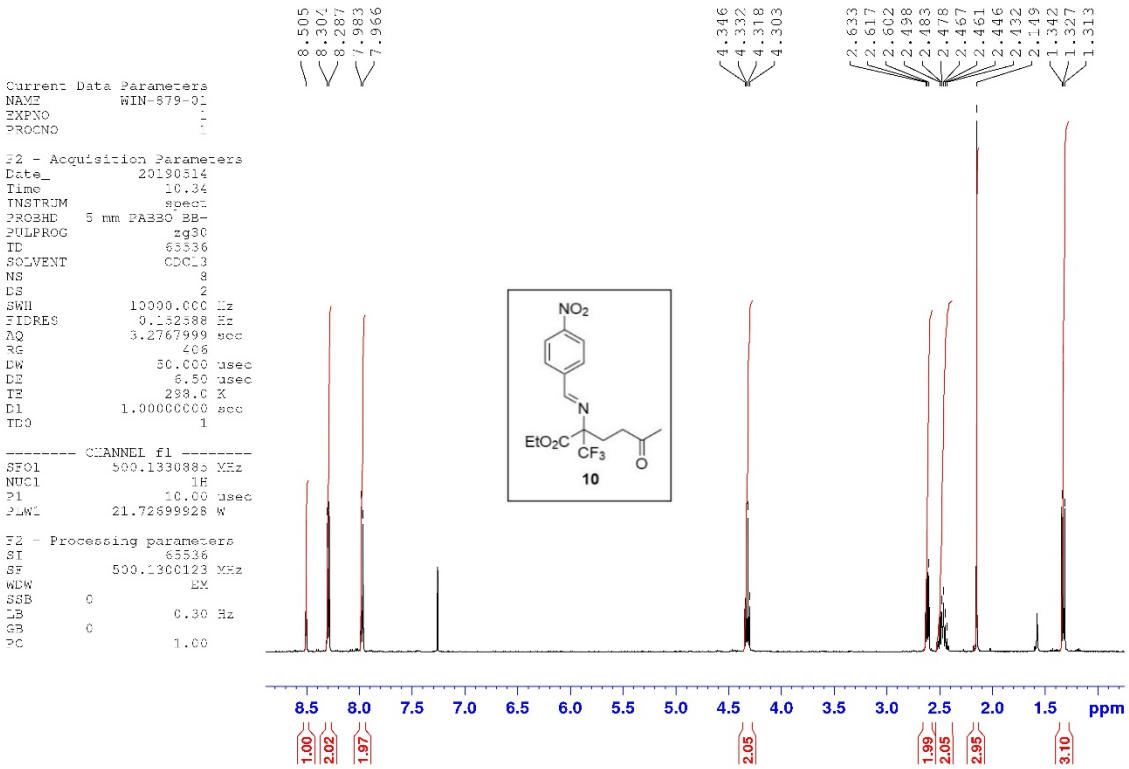

-63.179
-74.145
Current Data Parameters
NAME WIN-646-02
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190216
Time 11.09 h
INSTRUM spect
PROBHD Z862701_CC84 (
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 16
DS 2
SWH 66964.289 Hz
FIDRES 1.021794 Hz
AQ 0.9786710 sec
RG 724
DW 7.467 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 282.3761148 MHz
NUC1 19F
P1 8.60 usec
PLW1 19.99900055 W
F2 - Processing parameters
SI 65536
SF 282.4043550 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
CF3
F3C
H
N
CO2Et
CF3
O
O
5n
-60
-62
-64
-66
-68
-70
-72
-74
-76
-78
-80
ppm
5.57
3.00


Current Data Parameters
NAME WIN-846-02
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190216
Time 13.23 h
INSTRUM spect
PROBHD Z882/01_C064 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 27.73 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 8.88 usec
PLW1 50.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG_2 waltz16
PCPD2 90.00 usec
PLW2 20.00000000 W
PLW12 0.41727999 W
PLW13 0.20988999 W
F2 - Processing parameters
SI 32768
SF 75.4677393 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
199.061
198.878
166.419
142.526
141.853
136.921
136.521
136.240
135.792
132.809
132.041
131.595
129.997
129.081
128.379
128.461
126.879
124.683
123.373
123.260
123.117
122.255
121.062
74.743
74.374
71.353
69.384
63.370
61.163
54.650
13.309
5n
200
180
160
140
120
100
80
60
40
20
0
ppm


Current Data Parameters
NAME WIN-880-05
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190514
Time 13.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 812
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
-------- CHANNEL f1 --------
SFO1 500.1330885 MHz
NUC1 1H
P1 10.00 usec
PLW1 21.72699928 W
F2 - Processing parameters
SI 65536
SF 500.1300123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.493
7.487
7.467
7.461
7.455
7.309
7.302
7.296
7.290
5.325
5.317
4.488
4.406
3.955
3.941
3.934
3.926
3.919
3.912
3.905
3.891
3.578
3.564
3.557
3.548
3.542
3.535
3.528
3.514
3.406
3.398
0.789
0.775
0.761
8
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.05
6.49
2.30
1.15
1.09
1.22
1.21
1.11
3.00


-74.033
-71
-72
-73
-74
-75
-76
-77
-78
-79
ppm
3.00
8


167.564
134.779
133.841
133.230
130.882
130.620
130.108
129.460
129.282
129.200
127.643
125.219
122.962
113.209
112.058
74.793
74.574
70.392
63.766
57.758
48.725
13.241
200
180
160
140
120
100
80
60
40
20
ppm
8

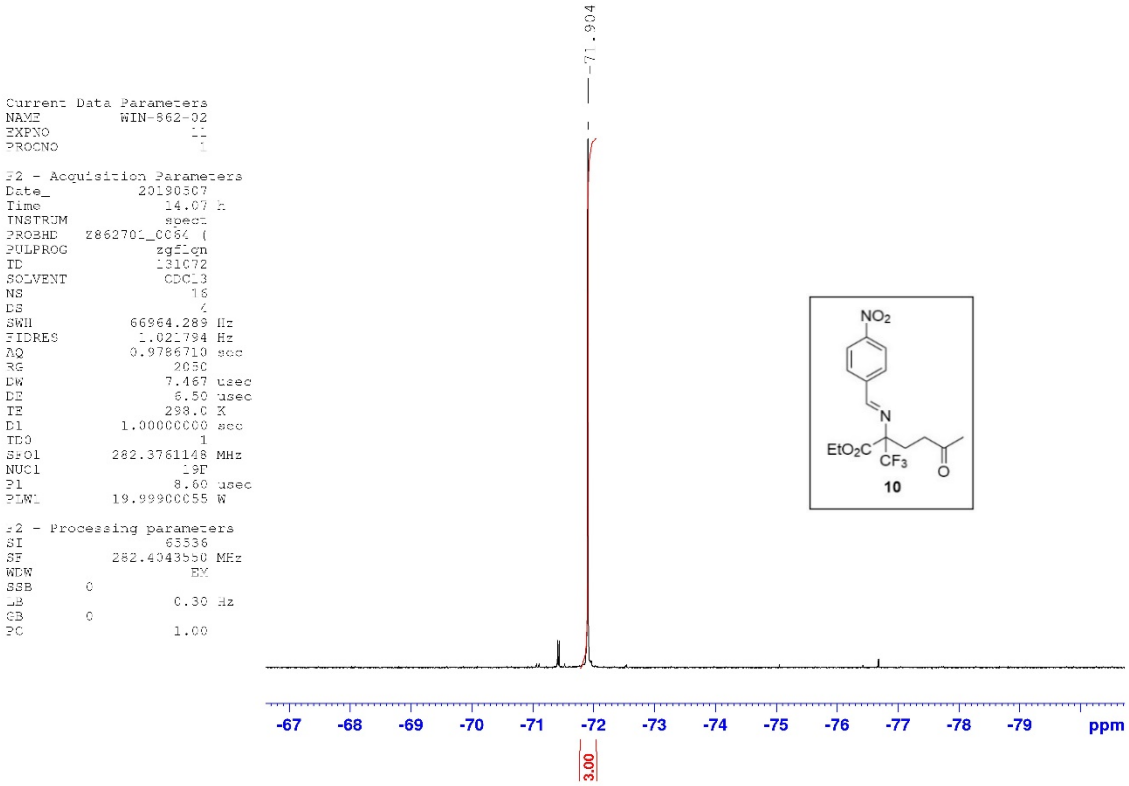



```
Current Data Parameters
NAME          WIN-879-01
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190514
Time              10.34
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                  406
DW               50.000 usec
DE                6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        500.1330885 MHz
NUC1                1H
P1                10.00 usec
PLW1        21.72699928 W

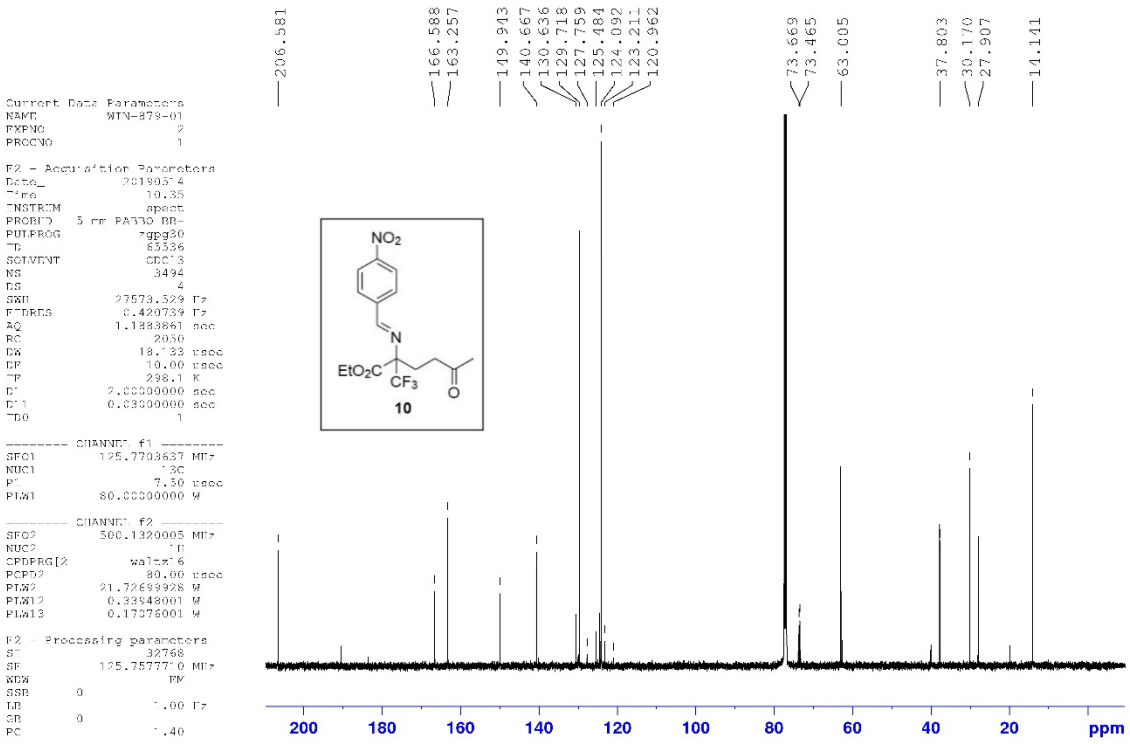
F2 - Processing parameters
SI                65536
SF          500.1300123 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```




```
Current Data Parameters
NAME          WIN-862-02
EXPNO                  11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190307
Time              14.07 h
INSTRUM           spect
PROBHD   Z862701_CC64 (
PULPROG          zgflqn
TD               131072
SOLVENT           CDCl3
NS                   16
DS                    4
SWH           66964.289 Hz
FIDRES        1.021794 Hz
AQ            0.9786710 sec
RG                 2050
DW                7.467 usec
DE                6.50 usec
TE                298.0 K
D1            1.00000000 sec
TD0                   1
SFO1        282.3761148 MHz
NUC1                19F
P1                8.60 usec
PLW1        19.99900055 W

F2 - Processing parameters
SI                65536
SF          282.4043550 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```




```
Current Data Parameters
NAME            WTN-279-01
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_          20190514
Time               10.35
INSTRM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3494
DS                    4
SWH           27573.529 Hz
FIDRES         0.420739 Hz
AQ             1.1883861 sec
RG                 2050
DW               18.133 usec
DE                10.00 usec
TE                298.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7703637 MHz
NUC1                 13C
P1                  7.50 usec
PLW1        80.00000000 W

======== CHANNEL f2 ========
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2        21.72699928 W
PLW12        0.33948001 W
PLW13        0.17376001 W

F2 - Processing parameters
SI                  32768
SF           125.7577710 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```